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# PROFILE: A GENERAL CODE FOR FITTING ION BEAM ANALYSIS SPECTRA

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ABERDEEN PROVING GROUND, MARYLAND

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A general program for analyzing energy distributions of particles scattered in ion beam experiments has been developed. This program uses numerical integration methods to model elastic scattering and nuclear reaction spectra from known cross sections, energy loss data and assumed depth concentration profiles of surface constituents. Direct comparison of the predicted and experimental distributions yields detailed, quantitative information about these depth concentration profiles in a complicated surface. The program is capable of analyzing all hydrogen

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or helium ion elastically scattered distributions and the (d,p) nuclear reaction peaks due to carbon, nitrogen, and oxygen. Analysis of the elemental concentration profiles of the surfaces of three different samples is discussed.

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# I. INTRODUCTION

Elastic and inelastic scattering of ion beams from solid surfaces has become a powerful analysis tool used to obtain a variety of information about such surfaces and thin films. Film layer thicknesses, concentrations of heavy atoms in light substrates and in many cases layer stoichiometries are obtainable from Rutherford backscattering (RBS) and nuclear reaction (NR) spectra. Chu, Mayer and Nicolet[1] have written a comprehensive book on the subject in which many formulae are derived relating basic data such as energy losses and cross sections to layer thicknesses and concentrations. For the most part, their discussions apply to situations where geometries are simple, layers are well defined and of uniform concentrations, and cross sections are Rutherford or constant.

In this report, a computer program which we have developed to model highly complex surfaces is discussed. A surface which may have many intermixed elements concentrated nonuniformly in depth, gradual interfaces between layers, small amounts of contaminants covering the outer surface or whose analysis depth is such that the probing cross section varies strongly, cannot be described by simple analytical expressions. In such complicated surfaces, all surface constituents contribute to the energy losses and the experimentally measured energy distributions are due to a complex folding of yields from all constituents. In addition, effects such as concentration gradients, energy loss straggling, and surface roughness can combine with the above factors to complicate the analysis even further.

The code generates the expected scattered particle spectra resulting from ion bombardment of the surface in such a way that a direct comparison to experimentally measured distributions can be made. The only variables in the calculation are the concentration profiles of all expected constituents of the surface. For this reason, it is necessary to have a prior knowledge of what elements make up the surface. Since only spectral shapes, not absolute magnitudes, are required for the fit, absolute quantities related to geometries and beam charge integrations need not be measured. However, the results are absolute in that the relative atomic percentages of the target constituents as a function of the depth in the surface are obtained. The basic data which are used in this calculation are cross-sections and energy losses of the projectiles in the target constituents and the ionization potentials of all elements.

A preliminary version of this code was described in reference 2. In that report, it was shown that the results obtained with shape fitting

1. W-K Chu, J.W. Mayer and M.A. Nicolet, Backscattering Spectrometry, Academic Press, New York, 1978.
2. A. Niiler, J.E. Youngblood, S.E. Caldwell and T.J. Rock, "An Accelerator Technique for the Study of Ballistic Surfaces", BRL Report No. 1815, August 1975. (AD #A016899)

were in excellent agreement with absolute measurements depending on precise geometry and beam charge integration. Many significant changes have since been incorporated into the calculation. They are of the type which make the program more general, provide up-to-date input data, allow for a more accurate determination of items such as energy loss straggling, or are of a housekeeping nature. The original version was operational on an SEL-86 computer but the current version runs on the ARRADCOM/BRL CDC-7600 machine.

In section II of this report, a description of the calculation is given and the function of each of the subroutines of the program is described. Sample calculations of three different surfaces are shown in section III. The appendices give the program listing as well as a description of the input cards.

## II. PROGRAM DESCRIPTION

This program calculates the yield as a function of energy resulting from a beam of hydrogen or helium ions backscattering or interacting with the constituents of a solid surface or thin film. A typical backscattering geometry is assumed where the incoming beam is defined by a set of apertures, the target can be set at any angle with respect to the beam and an energy dispersive particle detector is set at any angle behind an aperture. The target is divided into N layers (where $N \leq 100$) and each of the layers can be further subdivided into slabs if additional calculational resolution is desired. Each layer may contain up to five different elements (this number is easily increased); the concentration of each element is given in terms of relative atomic percent. Each layer is also assigned a thickness. The combination of layer thicknesses and atomic concentrations for the whole surface define the concentration profiles of the elements in the surface. The objective of the calculation is to arrive at a unique set of concentration profiles which yields the scattered particle energy distribution which best fits the experimentally measured distribution.

The calculation proceeds by allowing the incident beam to penetrate into the first layer of the surface. Figure 1 shows the beam, surface, detector geometry schematically. The energy in the layer (position x) is given by

$$E_i(x) = E_i(0) - \int_0^{x_1} \frac{dE_i(x')}{dx'}\, dx' \quad , \tag{1}$$

where $x_1 = x/\cos\phi$ and the energy loss in the layer is given by the Bragg additivity rule

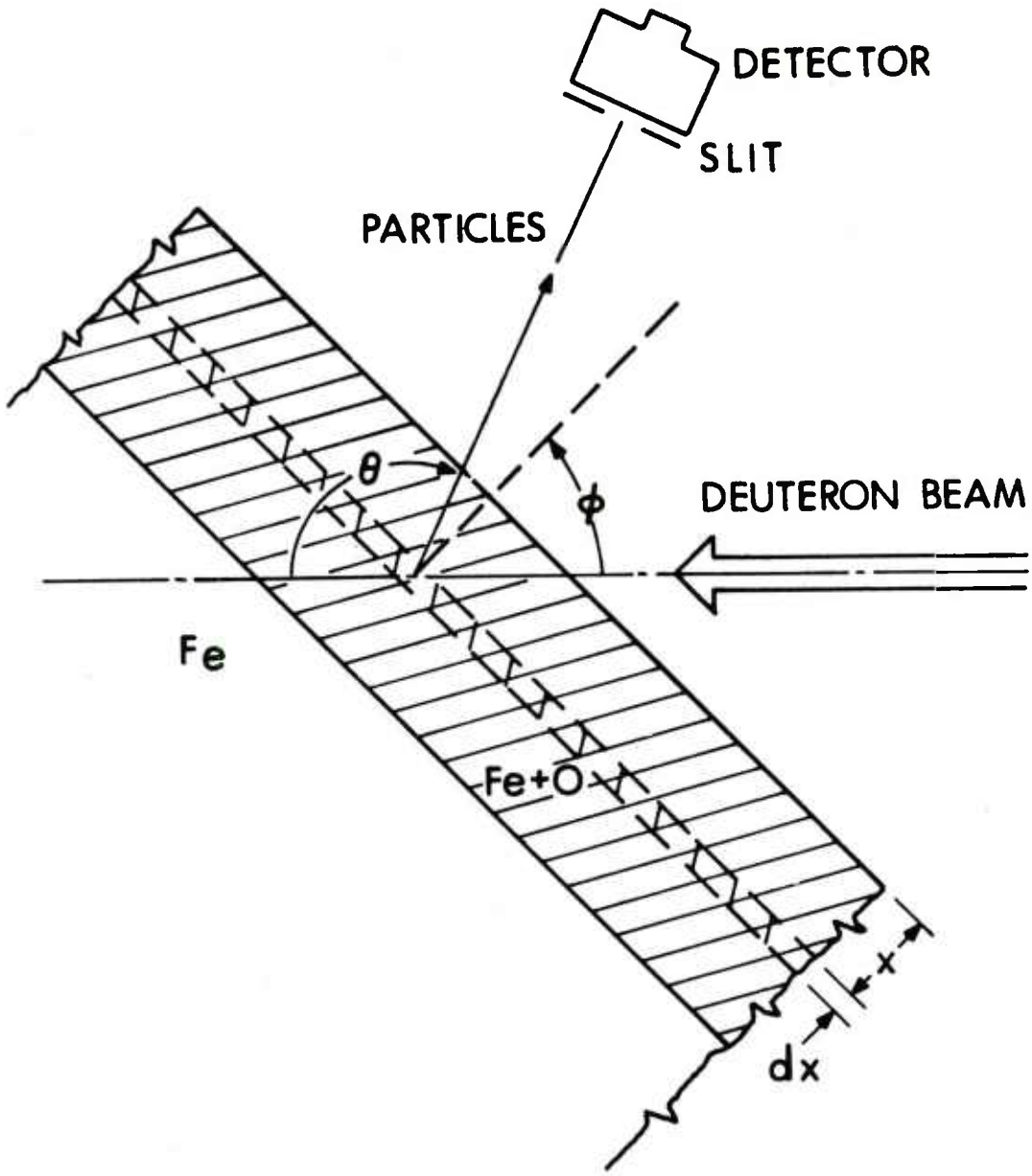


Figure 1. Beam Surface, Detector Geometry.

$$\frac{dE_i}{dx} = \sum_j f_j \frac{dE_i^j}{dx} \quad . \tag{2}$$

The $f_j$'s are the relative atomic percentages of the constituents and the $dE_i^j/dx$'s are the corresponding specific energy losses. The projectile then interacts with one of the layer constituents and either elastically scatters backward at angle $\theta$ or produces a reaction particle which is emitted at $\theta$. The probability of this interaction taking place is given by the cross section $\sigma(E_i(x),\theta)$. The outgoing particle energy is given by

$$E_o(x) = K\, E_i(x) \tag{3}$$

where K is the usual kinematic factor. As the outgoing particle now leaves the layer, it loses more energy so that its final energy becomes

$$E_f(x) = E_o(x) - \int_o^{x_2} \frac{dE_o(x')}{dx'}\, dx' \tag{4}$$

where $x_2 = x/\cos(\pi-\theta-\phi)$.

Gaussian energy broadening is applied at two points in this calculation. The $E_i(x)$ in equation 1 is broadened for beam energy resolution and energy loss straggling due to the incident energy loss. The resulting incident energy distribution Gaussian can be further divided into any number of energies, each centered at equal areas along the distribution. This procedure has the effect of treating the $E_i(x)$ distribution as if it consisted of many different energies, E, around $E_i(x)$, each having a scattering probability at x determined by the cross section, $\sigma(E)$. Each component of $E_i(x)$ is now scattered and followed out of the sample according to equations 3 and 4 and the final energy, $E_f(x)$, is broadened for energy loss straggling due to outgoing energy loss and detector resolution. The $E_f(x)$ Gaussians are now distributed into a final spectrum, each having been appropriately weighted by cross sections, layer thicknesses and constituent concentrations. Similar final energy distributions are obtained from all N layers of the surface while each layer is assumed to interact with the same number of incident particles, and the energies, energy losses and energy spreads are tracked. When the full, final distribution due to one surface constituent element is completed, the same procedure is followed for the other elements and

their contributions added to the final energy distribution at the proper energies with the proper weights. Additional calculations can be performed if the effects of two-dimensional geometries are important. This is usually the case if the beam spot or detector solid angle is unusually large.

The program proceeds to fitting the calculated distribution to an experimentally measured one. The two are fit by least squares methods, and the concentration profiles are adjusted and the full calculation run until a satisfactory fit is achieved. The primary criteria for acceptable fits are general agreement between the calculated and experimental shapes along with the lowest possible chi squared for the full calculation. The chi squared is given by

$$\chi^2 = \frac{1}{K-I} \sum_{i}^{N} (A \cdot Y_c(i) - Y_e(i))^2 / Y_e(i) \qquad (5)$$

where K is the number of points fit, I is the number of degrees of freedom, $Y_c$ is the calculated distribution, $Y_e$ is the experimental distribution and A is the least squares proportionality constant between the calculated and experimental distributions. Typically, I is given by

$$I = N\ (N_c - 1) \qquad (6)$$

where N is the number of layers used in the calculation and $N_c$ is the number of constituents per layer. Since usually it is possible to obtain an acceptable fit within five to ten iterations of the profiles by hand, no automatic search routine has been incorporated in this program. Computer costs would be driven up significantly by such auto-fit routines.

The primary functions of each of the program elements are:

(1) Program PROFILE. This is the control program. Inputs read by this section are the title, the reaction parameters, geometrical factors and surface layer configurations. It sets up the arrays of reaction parameters which determine the kinematic factors for each projectile - target constituent combination, determines whether the geometry is valid, follows the projectile energy losses both incoming and outgoing, and calls the various routines needed for some inputs, array setups and outputs.

(2) Subroutine SETION. This routine is used to calculate and set up the array of effective ionization potential ($I_{eff}$) for all layers. $I_{eff}$ is given by

$$\ln (I_{eff}) = \frac{\sum_i z_i f_i \ln (I_i)}{\sum_i z_i f_i} \qquad (7)$$

where $z_i$, $f_i$ and $I_i$ are the atomic number, percentage concentration and ionization potential respectively of the $i^{th}$ target constituent. The reference ionization potentials, $I_i$, are obtained from J.E. Turner[3].

(3) Subroutine SETTAB. This routine is used to input concentration information, set up tables of concentrations of the various elements in all layers and, when desired, calculate and output energy loss reference data as well as composite energy losses in all layers.

(4) Subroutine WIDTH. This routine calculates the energy loss straggling from the Bohr model using Lindhard and Scharff's correction factor for low and medium energy projectiles (see Reference 1). The straggling width is given by

$$\Omega^2 = \frac{W_m \cdot dE}{2 \cdot \ln \frac{W_m}{I_{eff}}} \cdot k \qquad (8)$$

where k = 1 for high energy projectiles and

$k = \frac{1}{2}\frac{4E}{I_{eff}}$ for intermediate and low energy projectiles. The numerical expression defining the line between high and intermediate energies as well as definitions of the other terms of equation 6 are given in section 2.6 of reference 1. A sense switch option permits the straggling width to be set to zero.

(5) Subroutines PICKE, FINDE, IGAUSS. These routines are used to calculate integrals of Gaussian distributions.

(6) Subroutine DIST. This routine builds the final energy distribution by summing all outgoing particle gaussian distributions weighted by the appropriate reaction cross section, target constituent concentration in the appropriate layer and that layer thickness. This distribution is built only between some preset minimum and maximum energies.

(7) Subroutine KIN. This routine calculates the non-relativistic two-body kinematics between an incoming and a particular target particle. It also calls the cross section routine and converts the cross section obtained into the laboratory system.

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3. J.E. Turner, "Studies in Penetration of Charged Particles in Matter", NAS-NRC Publication 11, Nuclear Science Series Report No. 39, (1962).

(8) Subroutine SIG. All reaction cross sections for a given reaction energy and angle are determined in this routine. If the reaction Q-value is zero, it automatically calculates the Rutherford cross section. However, in the case of proton elastic scattering from oxygen, the Rutherford cross section is modified by a factor obtained from Chow, et al.[4]. Otherwise, it must use stored arrays and interpolates for the cross section of interest. Currently, only the $^{12}C(d,p_o)$, $^{14}N(d,p_5)$ and $^{16}O(d,p_1)$ C.M. cross sections at 160° lab are stored. See references 5, 6 and 7 for the C,N and O cross sections respectively.

(9) Subroutine SHAPE. This routine calculates the mean energy and standard deviation of the energy as the incoming or outgoing particles traverse all but the final layer along their trajectories.

(10) Subroutine ELOSS. This routine calculates the energy loss of the Hydrogen or Helium isotopes through any given target. It uses the analytical expression

$$S = \sum_i f_i \frac{S_L^i \cdot S_H^i}{S_L^i + S_H^i} \tag{9}$$

where

$$S_L^i = A1(i) \cdot E^{AZ(i)} \tag{10}$$

and

$$S_H^i = \frac{A3(i)}{E} \ln\left(1 + \frac{A4(i)}{E} + A5(i) \cdot E\right) . \tag{11}$$

The $f_i$'s are the constituent concentrations, E is the particle energy and the A's are coefficients empirically determined by Anderson and

4. H.C. Chow, G.M. Griffiths and T.H. Hall, Can. J. Phys., 53 (1975) 1672.
5. M. Huez, L. Quaglia and G. Weber, "Fonction D'Excitation de la Reaction $^{12}C(d,p_o)^{13}C$ Entre 400 et 1350 keV - Distributions Angulaires", Nucl. Instr. Meth. 105 (1972) 197.
6. A. Niiler and R. Birkmire, "The $^{14}N(d,p_5)^{15}N$ Cross Section, 0.40-1.45 MeV", 4th International Ion Beam Analysis Conference, Aarhus, Denmark, June 25-29, 1979.
7. N. Longequeque, H. Beaumevieille, E. Ligeon, J.P. Longequeque, and M. Sandon, "Etude Des Reactions $^{16}O(d,\alpha_o)$, $^{16}O(d,p_o)$ et $^{16}O(d,p_1)$ de 300 keV a 1 MeV (Resultats Experimentaux), Le Journal de Physique, 26 (1965) 367.

Ziegler[8,9] for the $i^{th}$ target constituent. Equation 9 is the Bragg additivity rule for energy losses of composite materials.

(11) Subroutine OUTPUT. This routine inputs the experimental spectrum along with the calibration constants associated with it. It condenses the calculated spectrum, arranges it to match the experimental channel energies, calculates the least squares fit proportionality constant and the chi squared between the two spectra, and outputs a listing of the two normalized spectra.

(12) Subroutine PLOT1. This routine is used to output both experimental and calculated spectra on a line printer plot.

(13) Subroutine SWITCH. This routine is used to input sense-switches that control various calculations and outputs.

(14) Subroutine CONCTAB. This routine calculates and outputs the absolute concentration (in at/$cm^2$) of the various target constituents as a function of the target layer.

## III. SAMPLE CALCULATIONS

In this section, the results obtained using PROFILE in the analysis of three different surfaces are discussed. The first is a case where a well-polished, flat steel slab (FeO-7) was heated in air to oxidize the outer layers. The second shows results on a nozzle shaped steel surface (Nozzle 10) which was exposed to burning propellant gases at high temperatures ($T_V \sim 2400°k$) and pressures (170 MPa). These first two samples were prepared, bombarded with 0.665 MeV deuteron beams from the ARRADCOM/BRL Cockcroft-Walton accelerator and analyzed at BRL. The third sample, an anodized aluminum slab, was prepared and bombarded with 1 MeV protons and 2 MeV alphas by Simons et al.[10] of Naval Surface Weapons Center, White Oak, MD. The proton and alpha spectra were sent to BRL for analysis.

Figure 2 shows the concentration profiles for C,N,O and Fe which were required to produce the fits to the RBS distribution and NR peaks shown in figure 3. The carbon and oxygen profiles are surface peaked

8. H.H. Anderson and J.F. Ziegler, Hydrogen Stopping Powers and Ranges in All Elements, Pergamon Press, New York, 1977.
9. J.F. Ziegler, Helium Stopping Powers and Ranges in All Elements, Pergamon Press, New York, 1977.
10. D. Simons, private communication.

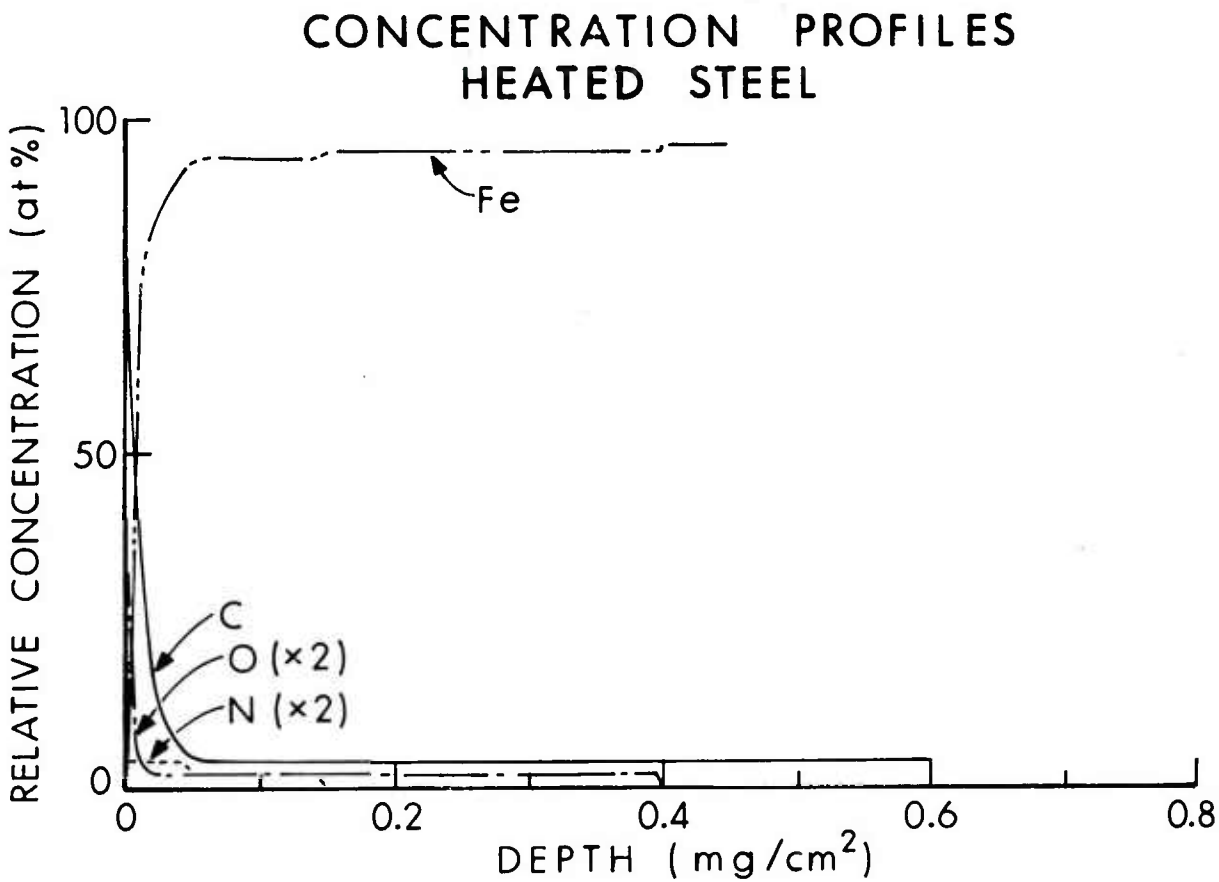


Figure 2. Concentration profiles for heated iron (FeO-7) slab.

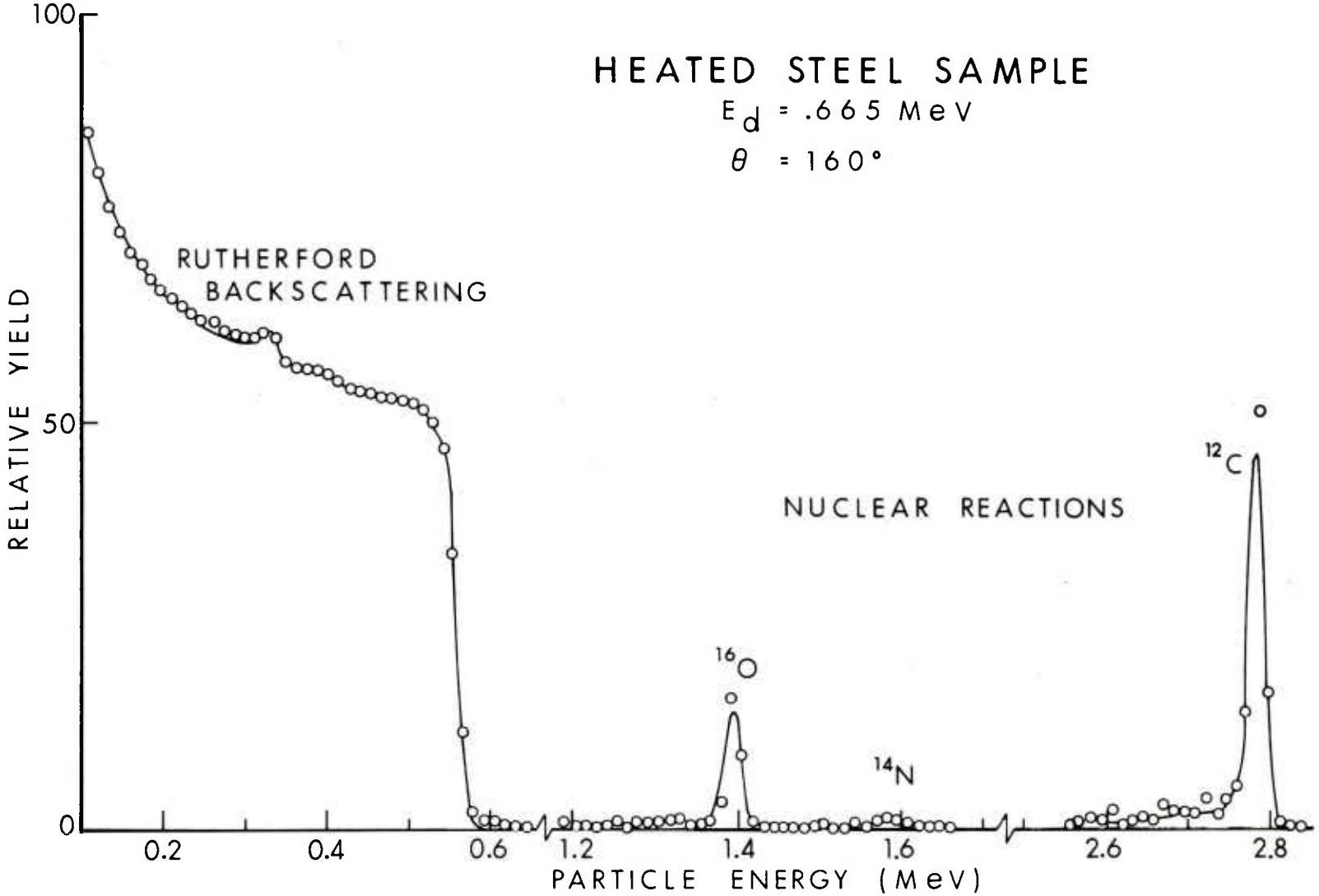


Figure 3. Fits to the Rutherford Backscattering and Nuclear Reaction peaks from sample FeO-7 using profiles shown in figure 2.

but they also extend into the sample the full 0.6 mg/cm$^2$ limit of the analysis capability with the .665 MeV deuterons. Upon closer examination, it can be seen that the carbon and oxygen together make up all but a few percent of the outermost 10 μg/cm$^2$ layer. The history of this sample helps explain this profile. The oxygen was introduced upon heating but the surface carbon resulted from vacuum system carbon being cracked onto the steel during beam bombardment. The fact that there is carbon at the 4% level all the way to 0.6 mg/cm$^2$ and oxygen at the 1% level to 0.4 mg/cm$^2$ is somewhat surprising and is most likely due to alloying impurity or recoil implantation. This sample has been used as a test sample for beam and electronics set ups for years. The original heating of the sample is the most probable cause of the relatively small amount of nitrogen that is found down to 150 μg/cm$^2$. The iron profile reflects the fact that the total atomic concentrations at all layers must equal 100% and that the full RBS distribution represents elastic deuteron yield from the outer .45 mg/cm$^2$.

Figures 4 and 5 show the concentration profiles and fits respectively to the steel nozzle exposed to the high temperature gases of burning propellant. As can be seen, all the profiles (C,N and O) are considerably different than what was found on simple heating of steel. Although the concentrations for C and O at the surface are still the highest, the surface peaks are not extremely sharp and the fall-off to the interior is much more gradual. In addition, there is a much larger concentration of nitrogen. It appears that the exposure has produced layers of oxides, carbides and nitrides in the steel surface extending as far as .5 to .6 mg/cm$^2$ into the surface. The consequences of such layer formation to the integrity of the surface upon succeeding exposures is currently being investigated.

The final sample is the anodized aluminum slab. Figure 6 shows the concentration profiles for H,C,O and Al that were needed to obtain the fits to the proton and alpha backscattering spectra shown in figures 7 and 8. The profiles for three different calculations are shown in figure 6.

The first calculation shown by the solid lines in figures 6, 7 and 8, gave the best fit. The whole 5 μg/cm$^2$ outer layer consisted of carbon, extending at lower levels to almost the 100 μg/cm$^2$ depth. Hydrogen was found at a constant 4% level throughout the oxide layer. Below the carbon surface layer, the oxygen/aluminum ratio is 58/38 which is consistent with $Al_2O_3$ stoichiometry of 60%-O, 40%-Al along with some of the oxygen being taken up by $H_2O$. In order to show the effect on the fit of a relatively minor change in the profiles, a calculation was done with the profiles indicated by the dot-dashed curves. These pro-

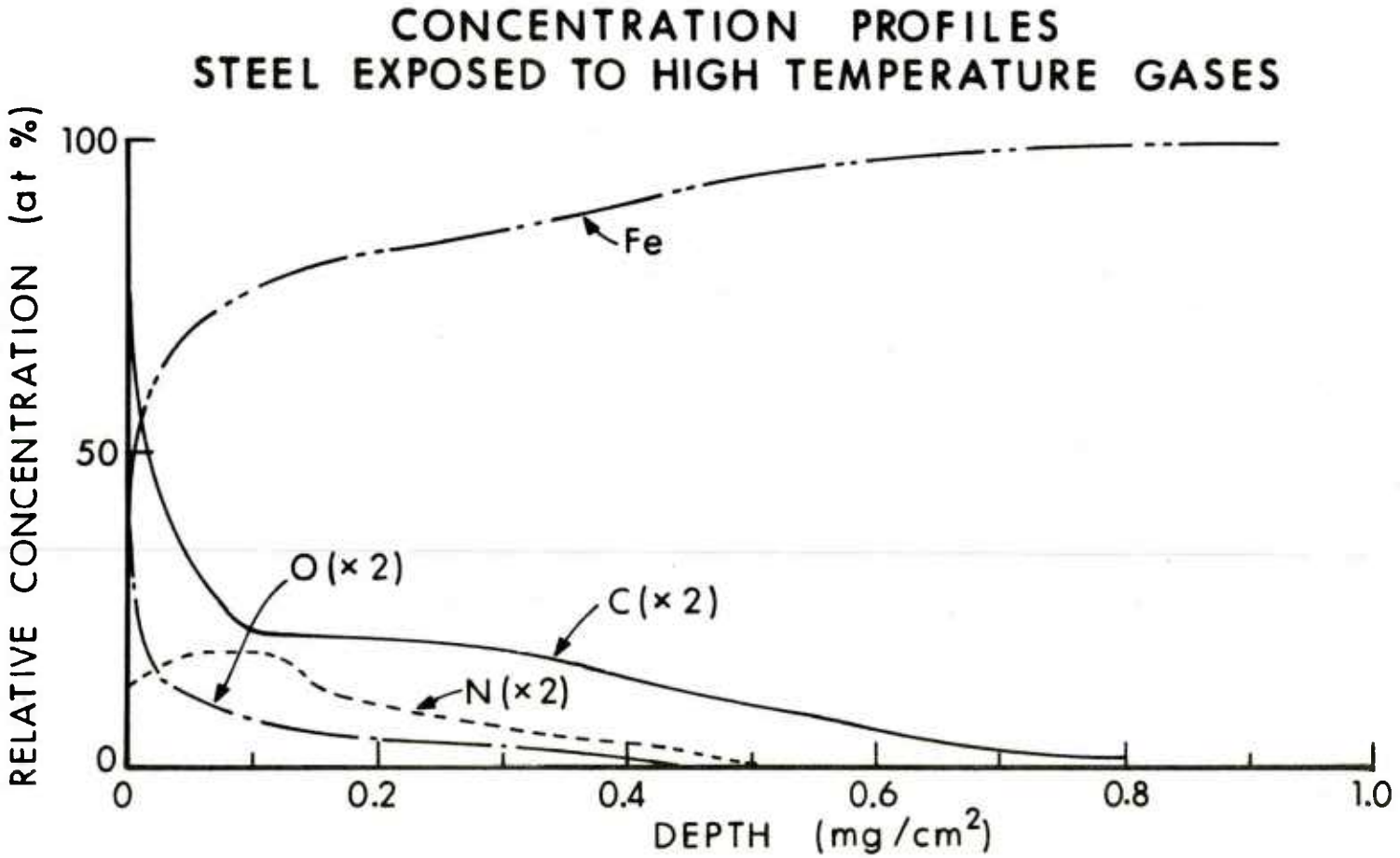


Figure 4. Concentration profiles for steel nozzle (Noz #10) exposed to high temperature propellant gases.

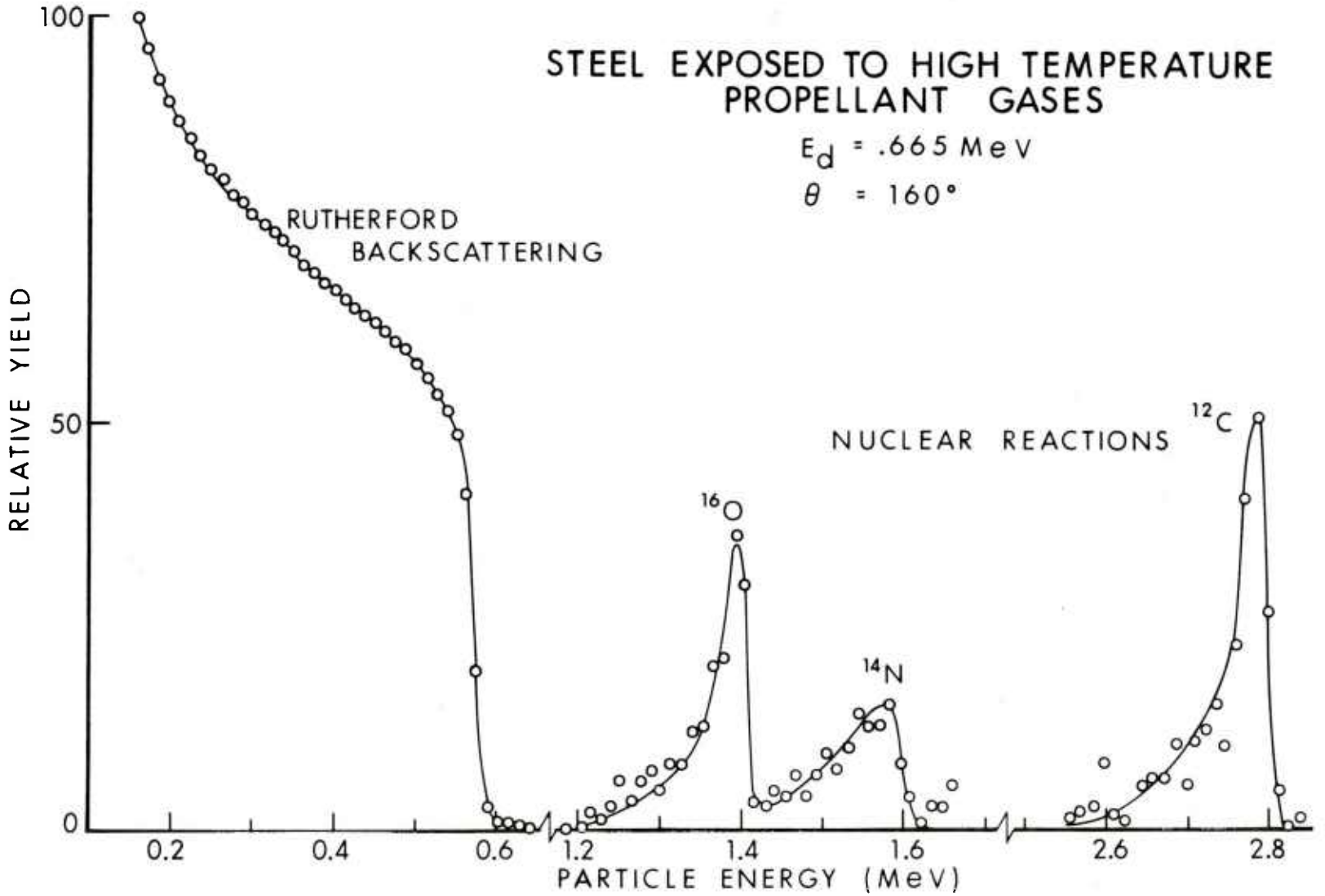


Figure 5. Fits to the RBS and NR peaks from Noz #10 using profiles shown in figure 4.

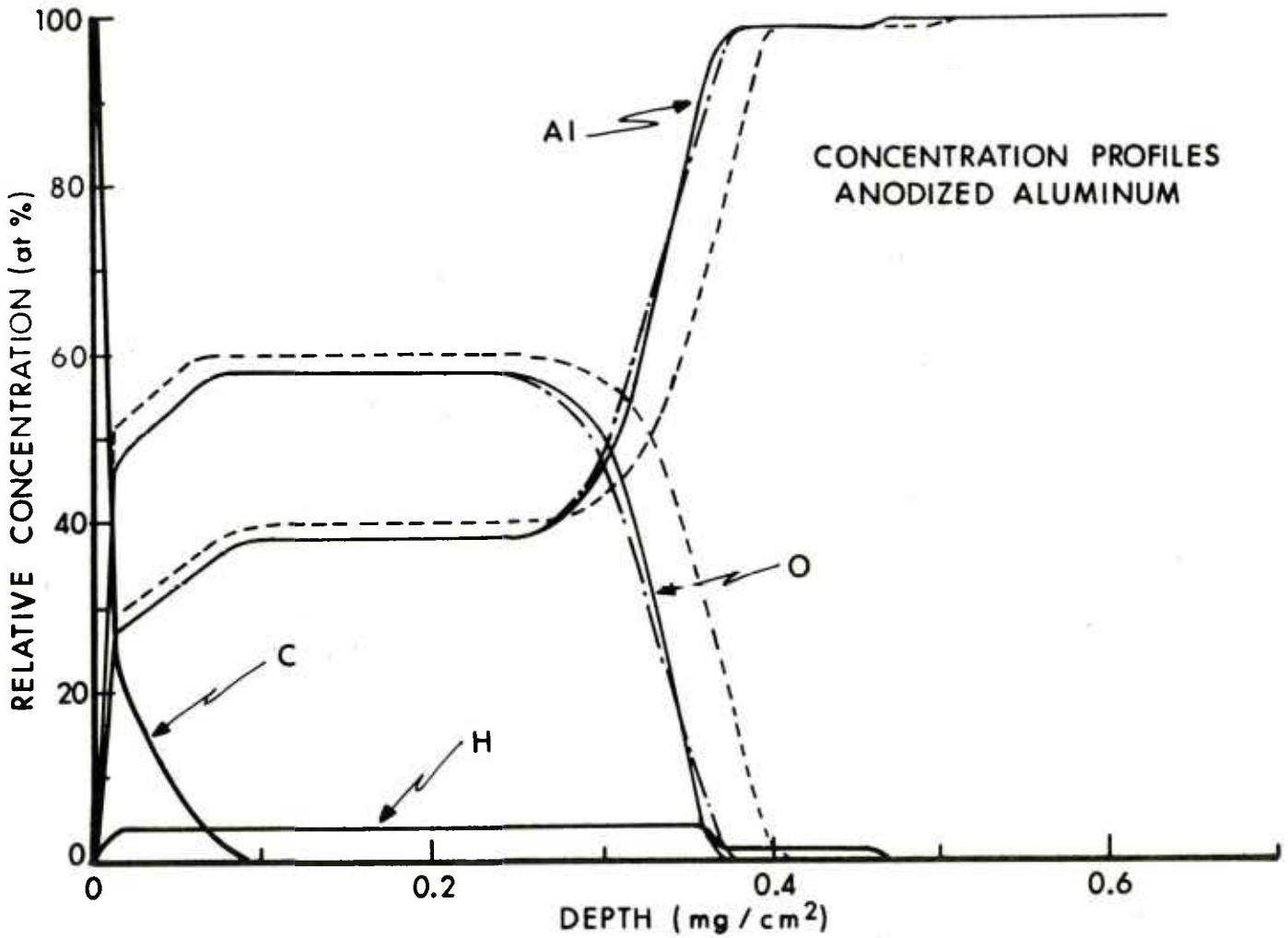


Figure 6. Concentration profiles for anodized aluminum sample. See the text for explanation of the different curves.

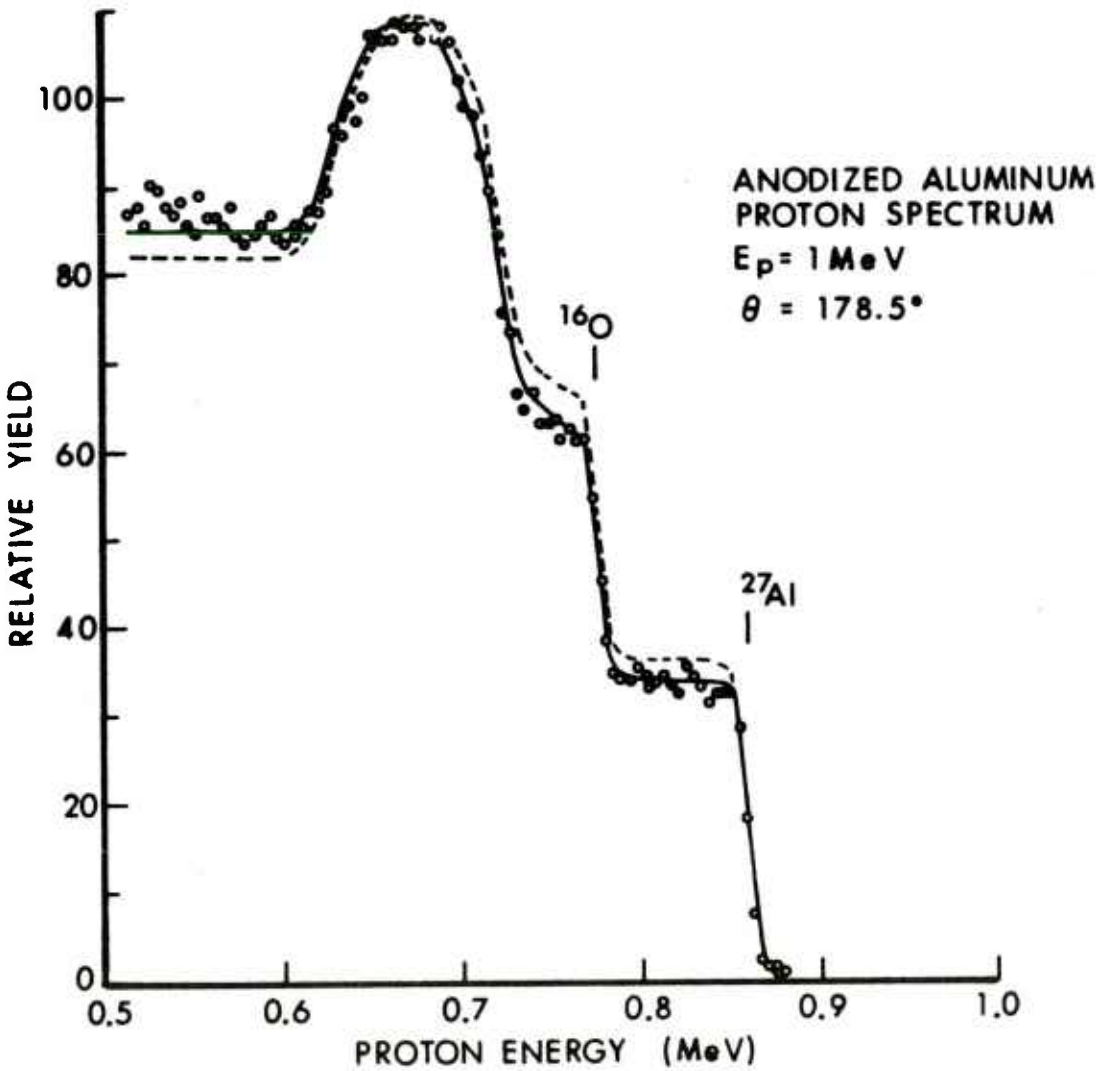


Figure 7. Fit to the proton RBS spectrum from the anodized aluminum sample using profiles shown in figure 6. See text for explanation of the two curves.

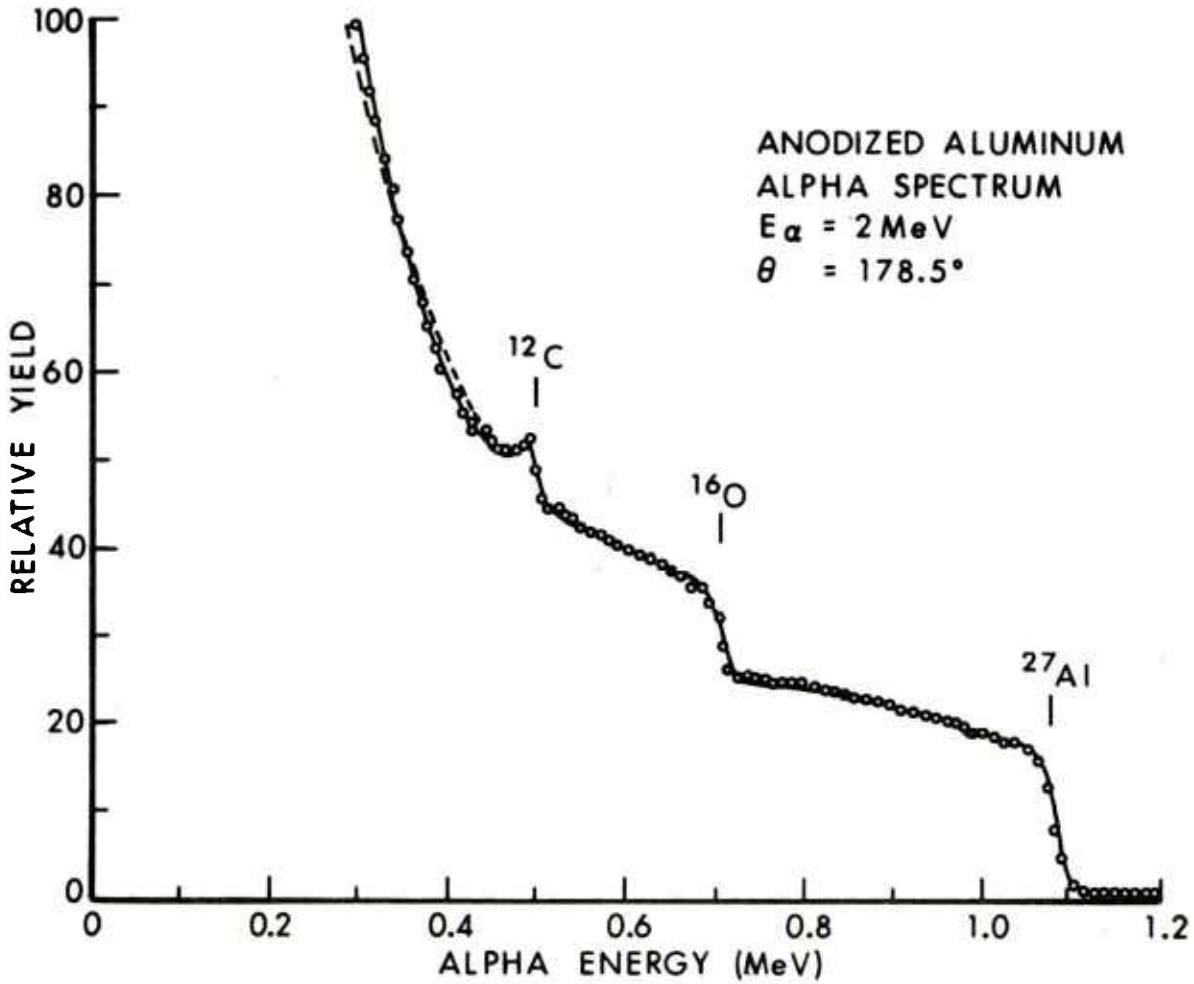


Figure 8. Fit to the alpha RBS spectrum from the anodized aluminum sample using profiles shown in figure 6. See text for explanation of the two curves.

files differ from the solid lines only in the oxide-metal interface and produce a discernable change in the fit only to the alpha spectrum and only in the region below 0.45 MeV. The combined chi-squared increased by 40% over the best fit value. The final calculation was done assuming no hydrogen at all in the oxide layer, shown by the dashed curves in figures 6, 7 and 8. The alpha spectrum was fit with a curve overlapping the solid line in all areas, but this set of profiles gave a fit to the proton spectrum which is quite poor in all areas. The combined chi-squared for this calculation increased by 15% over the best fit value. As in the case of the first calculation, the O/Al ratio is consistent with $Al_2O_3$ stoichiometry but the depth of the oxide layer is about 30 $\mu g/cm^2$ greater. This increased depth with no hydrogen is explained wholly by the hydrogen contribution to the stopping cross section.

Besides giving the generally good detail of the oxide layer and interface as described above, this analysis can also be used in determining the oxide layer density. However, such surface layer density determinations require separate measurement of the layer thicknesses by techniques such as optical or scanning electron microscopy, or electrochemical methods. The layer density is then given by $\rho=d/t$, where d is the layer areal density in $g/cm^2$ obtained by the ion beam methods described in this report and t is the layer thickness in cm. This type of density determination is currently being pursued for this anodized aluminum sample.

The concentration profiles shown in figures 2, 4 and 6 are actually stepwise functions in the numerical calculations. The step size varies over the calculation depth, being small where any concentration gradient is large and being large where all concentration gradients are small. For clarity of presentation, these stepwise functions are represented by smooth curves in all figures showing concentration profiles.

At this point, the question of uniqueness of the fits and absolute accuracies of the results will be discussed. As was pointed out, equally good fits to the alpha spectra of figure 7 could be obtained with different concentration profiles. This aspect of the analysis has been noticed with many other spectra. For this reason, it is necessary to fit more than one set of data with the same profile set. Thus, requiring the C,N,O peaks in the case of figures 3 and 5 and a fit to the proton spectrum in figure 7 adds considerably to the reliability of the results. To definitively test the uniqueness of a solution, a known standard sample should be analyzed, but this has not yet been done.

The absolute accuracies of both the concentrations and layer depths depend totally on the accuracy of the cross sections and stopping powers. Also as the layer thicknesses increase, uncertaintites in the theoretical expressions for energy loss straggling become more important,

especially in determining the interface profiles. The accuracies of stopping powers are presently in the range 5-10% so the layer thickness determination has a similar uncertainty. Typically, elastic cross sections have absolute uncertainties in the order 2-10% while reaction cross section uncertainties range from 10-20%. The statistics in the data also add to the error in the determination of concentrations. In the cases of the C,N and O reaction peaks, the statistics can produce 50% uncertainties in the concentration profiles in some regions. However, since those concentrations are in the range of a few atomic percent, those 50% uncertainties only amount to a few atomic percent error in the profiles. This result is generally borne out since the profiles usually need to be adjusted to within these limits for the best fits. In the cases where elastic distributions are fit, the cross section uncertainties dominate so that the errors are in the order of 2-10% or again a few atomic percent in the concentration profiles.

## IV. SUMMARY

A general and versatile program which was developed for obtaining concentration profiles of constituents of surface layers has been described. Its usefulness in defining, in great detail, both surface as well as interface structures has been demonstrated. Use of this analysis program on spectra generated by ion beam bombardments will aid in answering many detailed questions about surface layer stoichiometries, buildup of oxide, nitride or carbide layers, the extent of carburization of steel and in conjunction with optical measurements, the density of surface layers.

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# APPENDIX A - PROGRAM LISTING

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C     PROFILE -- PROGRAM TO ANALYZE BOTH RUTHERFORD BACKSCATTERING
C     AND NUCLEAR REACTION SPECTRA.  USES AVAILABLE VALUES OF CROSS
C     SECTIONS AND ENERGY LOSSES AND TAKES ENERGY RESOLUTIONS AND
C     STRAGGLING INTO ACCOUNT.  THE END RESULTS ARE DEPTH CONCENTRATION
C     PROFILES OF CONSTITUENTS OF THE SURFACE OR FILM IN ATOMIC PERCENT.
C     HISTORY OF THIS CODE -
C        1974 - ORIGINAL WRITTEN BY J.E.YOUNGBLOOD FOR SEL-86?
C        1975-76 - MODIFIED BY A.NIILER.
C        1977 - MODIFIED FOR CDC7600 BY J.GERRITS.
C        1978 TO NOW - CONTINUING MODIFICATION BY A.NIILER.
C     SUBROUTINE INFORMATION.
C     PROFILE - MAIN ROUTINE WHICH DIRECTS THE FLOW OF TRAFFIC. SETS
C        UP GEOMETRIES AND HAS MOST OF THE INPUTS.
C     SETTAB - INPUTS AND SETS UP CONCENTRATIONS. CAN OUTPUT ENERGY
C        LOSS TABLES FOR CHECKING PURPOSES.
C     SETION - CALCULATES IONIZATIONS POTENTIALS
C     WIDTH - CALCULATES ENERGY LOSS STRAGGLING
C     PICKE - PICKS ENERGY VALUES TO BE USED FROM GAUSSIANS
C     FINDE - NEEDED BY PICKE
C     DIST - DISTRIBUTES CALCULATED YIELD INTO FINAL ENERGY DISTRIBUTION
C     KIN - TWO BODY KINEMATICS CALCULATION
C     SIG - REACTION OR RUTHERFORD CROSS SECTIONS ARE DETERMINED
C        FROM TABLES OR CALCULATIONS
C     SHAPE - DETERMINES THE ENERGY AND ENERGY SPREAD OF PARTICLES
C        TRAVELING THROUGH SURFACE LAYERS
C     FLOSS - CALCULATES ENERGY LOSEES OF HYDROGEN AND HELIUM ISOTOPES
C        MODIFICATION NECDSSARY TO HANDLE OTHER TYPES OF PARTICLDS
C     OUTPUT - EXPERIMENTAL DATA INPUT. LEAST SQUARED FIT TO CALCULA-
C        TED DISTRIBUTION, BOTH ARRAYS PREPARED FOR OUTPUT
C     IGAUS - USED BY DIST
C     PLOT1 - LINE PRINTER PLOT OF EXPERIMENTAL AND CALCULATED DISTS
C     SWITCH - OUTPUTS SWITCH INFORMATION
C     CONCTAB - OUTPUT TABLE OF LAYER CONCENTRATIONS
C$    DEBUG
C$    ARRAYS
      PROGRAM PROFILE(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
     *DEBUG=OUTPUT)
      REAL M1,M2,M3,M4
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      COMMON/TABLES/ACO(5,100,2),CONCEN(5,100),CATARG(5,100),DFAC(100)
      COMMON /FLAGS/FLAG,FLAGA,FLAGB,FLAGC,FLAGD,FLAGE
        COMMON/SHA/NSLA(100),WT(100)
        COMMON/OU/X(410),Y(410),YY(410),XX(410)
      COMMON/S/ VALUE(2000),ISSW(10)
        COMMON/TIT/TITLE(20),NP
      COMMON/OEX/EMIN,EMAX
      DIMENSION THICK(100),FION(100),THKVAR(100)
        DIMENSION SM1(5),SM2(5),SM3(5),SM4(5),SQ(5),SEX(5)
        DIMENSION THKIN(100),THKOUT(100)
         INTEGER ZIN,ZTARG
      DATA FLAGCS/0.0/
C
    1 FORMAT(8F10.0)
    2 FORMAT(10I5)
    3 FORMAT(20A4)
11    FORMAT(1H1,25X,46HCALCULATION OF DEPTH PROFILE FROM THE SHAPE OF,
     *31H THE REACTION PRODUCT SPECTRUM ////
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```
     *15H REACTION DATA ,10X,20A4/
     *10X,4HM1 =,F10.6,10X,4HM2 =,F10.6,10X,4HM3 =,F10.6,10X,
     *4HM4 =,F10.6/
     *10X,19HREACTION Q-VALUE = ,F10.6,10X,19HEXCITATION ENERGY =,F10.5,
     *10X,13HNET Q-VALUE =,F10.5/
     *10X,13HBEAM ENERGY =,F10.5,22H MEV WITH A SPREAD OF ,F10.5,4HKEV /
     * 10X,14HTARGET ANGLE =,F10.3,15X,18HSCATTERING ANGLE =,F10.3/
     *10X,53HTHE REACTION PRODUCT DISTRIBJTION WILL BE STORED FROM,
     *F10.5,6HMEV TO,F10.5,3HMEV//
     *15H  GEOMETRY DATA//
     *10X,38HTHE BEAM-LIMITING SLIT HAS A RADIUS OF,F10.5,
     *10H CM.AND IS,F10.5,20H CM. FROM THE TARGET/
     *15X,35HTHE DEFINING SLIT IS REPRESENTED BY,I5,7H POINTS/
     *10X,25HTHE RADIUS OF THE BEAM IS,F10.5,18H CM. AT THE TARGET/
     *15X,28HTHE TARGET IS REPRESENTED BY,I5,7H POINTS/
     *10X,24HTHE DETECTOR APERTURE IS,F10.5,11H CM. AND IS,F10.5,
     *20H CM. FROM THE TARGET)
12    FORMAT(/,
     *15X,40HTHE DETECTOR APERTURE IS REPRESENTED BY=,I5,7H POINTS/
     *10X,22HDETECTOR RESOLUTION IS,F10.5,4H KEV//
     *13H TARGET DATA //
     *10X,45HTHE COMPOSITION OF THE TARGET IS DESCRIBED BY,I5,
     *32H LAYERS OF DIFFERENT COMPOSITION/
     *10X,35HTHE  FIRST LAYER IS SUBDIVIDED INTO ,I5,12HEQUAL SHEETS/
     *10X,58HTHE DISTRIBUTION OF INCOMING POINTS AT THE CENTER OF EACH ,
     *23HSHEET IS REPRESENTED BY,I5,19H OJTGOING PARTICLES//
     *34H THE COMPOSITION OF THE TARGET IS //
     *15X,10HIONIZATION,5(20H                ATOMIC)/
     *5X,5HLAYER,5X,11H POTENTIAL ,5(20H      ELEM   PERCENT)/)
171   FORMAT(/,5X,26HIMPOSSIBLE TARGET LOCATION,2X,16H ERROR GEOM EXIT)
  509 FORMAT(1H1)
511   FORMAT(12X,47H***   PARTICLE ENERGY SPECTRUM PARAMETERS   ***,21X,
     123H**   DEPTH PROFILE   **//
     *6X,3HEDO,6X,5HSUM-S,6X,3HEDX,7X,3HKIN,5X,6HSUM-SP,
     *7X,1HE,6X,6HSIGEDX,2X,4HRHOX,7X,5HDEPTH,12X,3HYTE/
     *5X,5H(MEV),5X,5H(MEV),5X,5H(MEV),15X,5H(MEV),5X,5H(MEV),3X,7H(MB/S
     *R),7X,8H(MG/CM2),3X,9H(MICRONS),7X,8H(AT/CM2))
512    FORMAT(6F10.4,F10.3,4X,F10.4,F13.5,E15.5)
  513 FORMAT(13HREAR OF LAYER,I4,F11.4,F13.4,F10.4,F44.5,F13.2,F17.5/
     *50X,37HOUTGOING PARTICLE CANNOT LEAVE TARGET/)
514   FORMAT(9X,5HLAYER,I4,F78.5,F13.2,F17.5)
 523  FORMAT(1H1)
526   FORMAT(1H0,38HREACTION IS DOUBLE-VALLED OR FORBIDDEN)
527   FORMAT(44H INCOMING OR OUTGOING PARTICLE GRAZES TARGET)
528   FORMAT(29H DETECTOR IS SHADOWED BY SLIT)
529   FORMAT(1H0,50HENERGY LOSS STRAGGLING CALCULATION IS NOT RELIABLE)
613   FORMAT(39HTOTAL CONCENTRATION OF TARGET COMPONENT,F8.2,1H=,E15.5,
     *7HAT/CN2.)
1000     FORMAT(3I5,5F12.5,1X,2(1PE12.5))
1111    FORMAT(8E12.5)
4771  FORMAT(8H THKVAR(,I5,4H) = ,F10.5,5H STOP)
C
 9991 READ(5,3)TITLE
      DO 141 I=1,100
141   THKVAR(I)=0.
      FLAGCS=1.0
      DTOR=3.141592654/180.
```

```
      A80 = 80.0*DTOR
C       INPUT DATA FOR CALCULATION OF CONSTANT
C       BEAM CHARGE IS GIVEN BY CHAR. DETECTOR SOLID ANGLE
C       GIVEN BY OMEGA.
        NCONS=0
        I=1
      CALL SWITCH
        READ(5,1) CHAR,OMEGA
410   READ(5,1)M1,M2,M3,M4,QREACT,EXCIT
      IF(M1.NE.0.)GO TO 414
      M1=SM1(I-1)$M2=SM2(I-1)$M3=SM3(I-1)$M4=SM4(I-1)
      QREACT=SQ(I-1)$EXCIT=SEX(I-1)$GOTO411
414   SM1(I)=M1
        SM2(I)=M2
        SM3(I)=M3
        SM4(I)=M4
        SQ(I)=QREACT
        SEX(I)=EXCIT
      Q=SQ(I)-SEX(I)
        I=I+1
        NCONS=NCONS +1
      GO TO 410
411    CONTINUE
C     M1,M2,M3,M4,QREACT DEFINE THE NUCLEAR REACTION
C     E IS THE ENERGY OF THE INCIDENT BEAM (MEV).
C     THETAT IS THE ANGLE BETWEEN BEAM AND TARGET NORMAL.
C     THETAD IS THE SCATTERING ANGLE FOR THE DETECTOR CENTER.
C     EXCIT IS THE EXCITATION ENERGY (MEV).
C     EMAX AND EMIN DEFINE THE LIMITING ENERGIES OF THE OUTPUT ARRAY.
C     DTHETA ALLOWS ANGULAR SPREAD OF OUTGOING PARTICLE TO BE FOLDED
C        INTO A CALCULATION
        READ(5,1)E,THETAT,THETAD,EMAX,EMIN,DTHET
C     RS AND DS ARE USED TO DEFINE DIVERGENCE OF BEAM.  IN THIS CASE,
C          THEY ARE TAKEN AS A FULLY ILLUMINATED QUADRUPOLE APERTURE.
C     RT IS THE TARGET RADIUS AT NORMAL INCIDENCE.  IN THIS CASE,
C          RT IS THE RADIUS OF THE ANTI-SCATTERING SLIT.
C     RD AND DD DEFINE THE DETECTOR LOCATION.
      READ (5,1) RS,DS,RT,RD,DD
C     NGS IS THE NUMBER OF POINTS USED TO DEFINE THE SLIT.
C     NGT IS THE NUMBER OF POINTS USED TO DEFINE THE TARGET.
C     NGD IS THE NUMBER OF POINTS USED TO DEFINE THE DETECTOR.
      READ(5,2)NGS,NGT,NGD
C     DETRES IS THE DETECTOR RESOLUTION IN KEV
C     ERES IS THE BEAM ENERGY RESOLUTION IN KEV
      READ(5,1)DETRES,ERES
C     NLAYER IS THE NUMBER OF LAYERS IN THE TARGET. LIMITED TO 100.
C     NSLAB IS THE NUMBER OF SECTIONS OF THE FIRST TARGET LAYER.  ALL
C        SUBSEQUENT LAYERS WILL HAVE SLABS OF THE SAME THICKNESS.
C        THIS IS DONE IN 4730 LOOP.
C     NDIV IS THE NUMBER OF POINTS USED TO REPRESENT THE GAUSSIAN SHAPE
      READ(5,2)NLAYER,NSLAB,NDIV
      IF(NLAYER.GT.100) NLAYER=100
      IF (NSLAB.GE.100) NSLAB=100
      ANGD=THETAD*DTOR
      ANGT=THETAT*DTOR
      IF(ISSW(4).NE.1) GO TO 5
      WRITE(6,11)TITLE,M1,M2,M3,M4,QREACT,EXCIT,Q,E,ERES,THETAT,THETAD,
```

```
     *EMIN,EMAX,RS,DS,NGS,RT,NGT,RD,DD
      WRITE(6,12)NGD,DETRES,NLAYER,NSLAB,NDIV
    5 CONTINUE
C     INPUT THE CONCENTRATION DATA AND GET ENERGY LOSS INFORMATION
C        OUTPUT IF ISSW(1)=1
      CALL SETTAB(NLAYER,THICK,FION)
C
C     PROGRAM RETURNS HERE AT COMPLETION OF OUTPUT.
C
C     INITIALIZE THE OUTPUT ARRAY 'VALUE'.
      CALL OUT1
C     THICK IS THE ACTUAL THICKNESS OF EACH LAYER IN MG/CM**2
C
C     USE A NEGATIVE VALUE OF THICK(1) TO INITIATE OUTPUT OF DATA.
C          ONLY ONE CARD NEED BE USED TO FLAG OUTPUT EVEN IF NLAYER
C               EXCEEDS 8.
      READ(5,*)(THICK(I),I=1,NLAYER)
C    *    *    *    *    *    *    *    *    *    *    *    *    *    *
      DO 30 I=1,NLAYER
 30   THKVAR(I)=0.0
C     NO THICKNESS VARIATION IS ALLOWED AS OF 12DEC78.  THESE FEW
C     CARDS NEED TO BE UPDATED  SHOULD TOE NEED ARISE TO START AGAIN
C     WITH SURFACE ROUGHNESS CALCULATIONS)
C    *    *    *    *    *    *    *    *    *    *    *    *    *    *
      DO 4730 ISLA=1,NLAYER
        II= ISLA +1
      IF(THKVAR(II).NE.0.)WRITE(6,4771)II,THKVAR(II)
 4730 NSLA(ISLA)=THICK(ISLA)/THICK(1)*NSLAB
      IF(THKVAR(1).NE.0.)NSLA(1)=1
      NSLAA=NSLAB
C
      IF(ISSW(6).NE.0)WRITE(6,523)
C     BEGIN COMPUTATION
C
      FLAG=0.0
      FLAGA=0.0
      FLAGB=0.0
      FLAGC=0.0
C     FLAG NOT 0 INDICATES THE REACTION CANNOT OCCUR OR IS DOUBLE-VALUED
C     FLAGA NOT 0 INDICATES THAT INCOMING OR OUTGOING PARTICLE GRAZES TARGET
C     FLAGB NOT 0 INDICATES SHADOWING OF DETECTOR BY SLIT
C     FLAGC NOT 0 INDICATES THE GAUSSIAN WIDTH IS NOT RELIABLY CALCULATED
        NIX=2.*DTHET+1
        DTHET=DTHET*DTOR
        ANGT = ANGT -DTHET
        DO 600 MULT = 1,NIX
        XMULT=MULT-1
        ANGT = ANGT + XMULT * DTOR
      DO 500 IGS=1,NGS
C     SELECT A POINT IN THE SLIT.
      XS=DS
      YS=0.
      IF(NGS.LT.2) GO TO 51
      YS=RS*(1.-2.*FLOAT(IGS-1)/FLOAT(NGS-1))
   51 CONTINUE
      DO 500 IGT=1,NGT
C     SELECT A POINT IN THE TARGET.
```

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      XT=YT=0.
      IF(NGT.LT.2) GO TO 52
      XT=RT*SIN(ANGT)*(2.*FLOAT(IGT-1)/FLOAT(NGT-1)-1.)
      YT=RT*COS(ANGT)*(1.-2.*FLOAT(IGT-1)/FLOAT(NGT-1))
C     THE NEXT 2 STATEMENTS ASSUME RT IS 'DEFINED' BY BEAM SIZE.
      XT=XT/COS(ANGT)
      YT=YT/COS(ANGT)
   52 CONTINUE
      DO 500 IGD=1,NGD
C     SELECT A POINT IN THE DETECTOR APERTURE.
      XD=-DD*COS(ANGD)
      YD=DD*SIN(ANGD)
      IF(NGD.LT.2) GO TO 53
      XD=-DD*COS(ANGD)+RD*SIN(ANGD)*(2.*FLOAT(IGD-1)/FLOAT(NGD-1)-1.)
      YD=DD*SIN(ANGD)+RD*COS(ANGD)*(2.*FLOAT(IGD-1)/FLOAT(NGD-1)-1.)
   53 CONTINUE
      IF(XS.LE.XT) GO TO 170
      YDA=YT+(RS-YT)*(XD-XT)/(DS-XT)
      IF(YD.LE.YDA) GO TO 180
      GEOA=(XT-XS)**2+(YT-YS)**2
      GEOB=(XT-XD)**2+(YT-YD)**2
      GEOC=(XD-XS)**2+(YD-YS)**2
      U=GEOA+GEOB-GEOC
      U=U*0.5/SQRT(GEOA*GEOB)
      ANGLAB=ACOS(AMIN1(U,1.))
      ANGLAB=3.14159-ANGLAB
      ANGIN=ANGT-ATAN((YS-YT)/(XS-XT))
      ANGOUT=3.141592654-ANGLAB-ANGIN
      DEGLAB=ANGLAB/DTOR
      DEGIN=ANGIN/DTOR
      DEGOUT=ANGOUT/DTOR
C     GEOMETRIC PARAMETERS HAVE BEEN DEFINED FOR IGS,IGT,AND IGD.
C
C     TEST FOR VALID GEOMETRY
      IF (ANGIN.LT.A80.AND.ANGOUT.LT.A80) GO TO 100
C     PARTICLE ENTERS OR LEAVES WITHIN 10 DEGREES OF SURFACE PLANE.
C     FLAG GRAZING INCIDENCE AND SKIP.
      FLAGA=1.0
      GO TO 500
  170 WRITE(6,171)
C     BAD GEOMETRY FOUND.
      STOP
  180 CONTINUE
C     DETECTOR SHADOWED BY SLIT.  FLAG AND SKIP.
      FLAGB=1.0
      GO TO 500
C
C     GEOMETRY IS VALID.
C
100   CONTINUE
      U=1.0/COS(ANGIN)
      V=1.0/COS(ANGOUT)
      DO 110 I=1,NLAYER
      THKIN(I)=THICK(I)*U
110   THKOUT(I)=THICK(I)*V
      IF(THKVAR(1).EQ.0.) GO TO 7878
      THKIN(1)=0.5*THKIN(1)
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      THKOUT(1)=0.5*THKOUT(1)
7878  CONTINUE
      WIDT=0.
      DO 498 KM=1,NCONS
        M1=SM1(KM)
        M2=SM2(KM)
        M3=SM3(KM)
         M4=SM4(KM)
      IF(M2.EQ.0)GO TO 498
        Q=SQ(KM)-SEX(KM)
      DO 499 LLAYER=1,NLAYER
      LAYER=LLAYER
      IF(CONCEN(KM,LAYER).LE.0.)GOTO499
C     EA IS THE MEAN ENERGY AND WID IS THE STANDARD DEVIATION OF THE
C          INCIDENT BEAM ENERGY DISTRIBUTION.
C     INITIALIZE EA AND WIDSQ FOR THIS LAYER.
      CALL SHAPE(E,DE,WID,M1,1,FION,THKIN,THKVAR,LAYER)
      IF(E.LE.DE)GOTO499
      EA=E-DE
      EA0=EA
      WIDSA=0.
C     EA0 IS THE ENERGY OF THE INCIDENT PARTICLE AS IT ENTERS THE LAYER
      WIDSQ=WID**2 + WIDT
      THKB=0.0
        UA=1.
      NSLAB=NSLA(LAYER)
      THKN=THKIN(LAYER)/NSLAB
C     EACH LAYER OF INTEREST IS DIVIDED INTO NSLAB SLABS.
      IF(LAYER.EQ.1.AND.THKVAR(LAYER).NE.0.)GO TO 4177
      GO TO 4178
C     SKIP TO ST 4178 IF NO SURFACE ROUGHNESS IS USED.
4177  LAYER=2
C      *    *    *    *    *    *    *    *    *    *    *    *    *
C     THIS REGION TO BE USED IF SURFACE ROUGHNESS CALCULATION DONE AGAIN
C      *    *    *    *    *    *    *    *    *    *    *    *    *
 4178     CONTINUE
      DO 300 NS=1,NSLAB
      THKA=THKN*UA
      THKB=THKB+THKA
      CALL ELOSS(EA,LAYER,1,THKA,DE)
      IF(EA.LE.DE)GOTO499
      CALL WIDTH(EA,DE,M1,FION(LAYER),WIDA,LAYER)
      WIDSA=WIDSA+WIDA**2
          EA=EA-DE
      WID=WIDSA + WIDSQ +(ERES*.001)**2
C     THE INCIDENT BEAM NOW HAS A GAUSSIAN DISTRIBUTION(EA,WID).
      WID=SQRT(WID)
C
C     THE INCIDENT PARTICLE HAS REACHED THE REACTION SITE.
C
C     REPRESENT THE DISTRIBUTION BY SELECTING NDIV ENERGIES SUCH THAT
C      THE INTEGRAL OF THE DISTRIBUTION FROM ONE ENERGY TO THE NEXT
C          YIELDS A CONSTANT AREA.
      DO 200 ND=1,NDIV
      UB=(FLOAT(ND)-0.5)/FLOAT(NDIV)
      UB=1.0-UB
C     SELECT NDIV REPRESENTATIVE ENERGIES SUCH THAT THE INTEGRAL
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```
C      OF THE DISTRIBUTION FROM -INFINITY TO E EQUALS  1 - (N-1/2)/NDIV.
       CALL PICKE (UB,EA,WID,EB)
C      THE REACTION NOW OCCURS.  THE OUTGOING PARTICLE HAS AN ENERGY EC.
          CALL KIN(EB,ANGLAB,EC,XSEC,KM)
       IF(XSEC.LE.0.0) GO TO 300
C      THE DISTRIBUTION OF THE OUTGOING PARTICLE IS NOW DETERMINED AS IT
C           TRAVERSES THE SAMPLE.
       THKC=THKA*THKOUT(LAYER)/THKIN(LAYER)
       WIDSQB=0.
       DO 402 KK=1,NS
       CALL ELOSS(EC,LAYER,2,THKC,DE)
       IF(EC.LE.DE) GO TO 300
       CALL WIDTH(EC,DE,M3,FION(LAYER),WIDB,LAYER)
       WIDSQB=WIDSQB+WIDB**2
       EC=EC-DE
 402     CONTINUE
C      THE REACTION PRODUCT HAS LEFT THE LAYER IN WHICH THE REACTION
C           OCCURRED.
       ED=EC
       CALL SHAPE(ED,DE,WIDB,M3,2,FION,THKOUT,THKVAR,LAYER)
       IF(ED.LE.DE) GO TO 300
       WIDSQB=WIDSQB+WIDB**2
        IF(NDIV.EQ.1)WIDSQB=WIDSQB+WID**2
C      INCREASE WIDB TO INCLUDE THE EFFECT OF DETECTOR RESOLUTION.
       WIDB=SQRT(WIDSQB+(0.001*DETRES)**2)
       EE=ED-DE
       GO TO 3178
C       *    *    *    *    *    *    *    *    *    *    *    *    *
C      AGAIN, STUFF RELATED TO SURFACE ROUGHNESS REMOVED
C       *    *    *    *    *    *    *    *    *    *    *    *
 3178     CONS=CHAR*OMEGA*3.906*(10.0**6)
          WEIGHT=XSEC * CONCEN(KM,LAYER)*THKN*CONS
C      THKN IS THE SLANT RANGE THROUGH THE SLAB FOR THE INCIDENT BEAM.
C      THE DISTRIBUTION OF THE OUTGOING PARTICLE AT THE DETECTOR IS
C           GAUSSIAN (EE,WIDB).
C      THE RELATIVE WEIGHT OF THIS DISTRIBUTION IS 'WEIGHT'.
C      THE DISTRIBUTIONS ARE ACCUMULATED IN THE OUTPUT ARRAY'VALUE'.
       CALL DIST(EE,WIDB,WEIGHT,EMAX,EMIN)
       IF(ISSW(6).NE.1.OR.EE.LT.EMIN)GO TO 200
         WRITE (6,1000)LAYER,NS,ND,EA,WID,EE,WIDB,
     $ CONCEN(KM,LAYER),WEIGHT,XSEC
200        CONTINUE
300        CONTINUE
499    CONTINUE
498    CONTINUE
500    CONTINUE
  600     CONTINUE
       IF(ISSW(10).EQ.1)CALL CONCTAB(NLAYER,THICK)
         NSLAB=NSLA(1)
         NP=0
       CALL OUTPUT(YMX)
       CALL OUT2
C      THE PUBLIC RELATIONS BLURB HAS BEEN REMOVED DUE TO RELATIVELY
C         NONSENSICAL INFORMATION CONTAINED THEREIN.
C      OUTPUT FLAGS
       WRITE(6,523)
       IF(FLAG.GT.0.1) WRITE(6,526)
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      IF(FLAGA.GT.0.1) WRITE(6,527)
      IF(FLAGB.GT.0.1) WRITE(6,528)
      IF(FLAGC.GT.0.1) WRITE(6,529)
      READ(5,2)I
      IF(I.NE.0)GO TO 9991
      STOP
      END



      SUBROUTINE SETION(Z,FION,N)
C
C     THIS SUBROUTINE CALCULATES THE EFFECTIVE IONIZATION POTENTIAL
C
      INTEGER Z
      REAL ION
      COMMON/SET/ATARG(5,100),ATMASS(100)
      DIMENSION ION(100),Z(1)
      DATA(ION(I),I=1,94)/18.5,42.0,37.8,66.8,73.0,77.5,84.7,88.8,121.0,
     *131.0,143.0,152.4,162.5,172.2,181.5,192.0,200.6,208.8,218.5,228.0,
     *237.3,246.4,255.3,265.2,275.0,284.7,294.3,304.1,313.8,324.0,333.9,
     *343.7,353.1,362.1,371.0,380.9,390.7,400.5,410.3,420.0,429.7,439.3,
     *448.9,458.5,468.0,477.9,487.8,497.7,507.6,517.5,527.3,537.2,547.0,
     *556.7,566.5,576.2,586.0,595.7,605.3,615.0,624.6,634.3,643.9,653.4,
     *663.0,672.9,682.7,692.6,702.4,712.3,722.1,731.9,741.7,751.5,761.3,
     *771.0,780.8,790.5,800.3,810.0,819.7,829.4,839.1,848.8,858.5,868.2,
     *877.8,887.5,897.1,906.8,916.4,926.0,935.6,945./
      U=V=W=0.0
      DO 10 I=1,5
      IF(ATARG(I,N).LT.0.0001)GO TO 10
      J=Z(I)
C     THE DENSITY IS PROPORTIONAL TO A(I), THE RELATIVE WEIGHT OF A
C          CONSTITUENT.
      X=FLOAT(J)*ATARG(I,N)/ATMASS(J)
      U=U+X
      W=W+X*ALOG(ION(J))
   10 CONTINUE
      W=W/U
      FION=EXP(W)
      RETURN
      END
```

```
      SUBROUTINE SETTAB(NLAYER,THICK,FION)
C     THIS SUBROUTINE INPUTS AND SETS UP THE CONCENTRATION TABLES AND
C        CALCULATES AND OUTPUTS ENERGY LOSS TABLES FOR CHECKING PURPOSES
C        ISSW(1) HAS TO BE 1 TO GET THIS ELOSS OUTPUT.  SEE THE
C        DESCRIPTION IN FRONT OF ELOSS SUBROUTINE FOR HOW ENERGY
C        LOSSES ARE CALCULATED.
      COMMON/TABLES/ACO(5,100,2),CONCEN(5,100),CATARG(5,100),DFAC(100)
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      COMMON/S/VALUE(2000),ISSW(10)
      COMMON/TSYMB/SYMB(100),ICON
      COMMON/SET/ATARG(5,100),ATMASS(100)
      COMMON/ELO/IZA
      DIMENSION THICK(100),FION(100),EREF(37),DUMT(100),S1(5,37,2)
      DIMENSION S2(15),ARA(1000)
      INTEGER SYMB,ZIN,ZTARG
      REAL M1,M2,M3,M4
      DATA SYMB/2H H,2HHE,2HLI,2HBE,2H B,2H C,2H N,2H O,
     12H F,2HNE,2HNA,2HMG,2HAL,2HSI,2H P,2H S,2HCL,2H A,2H K,2HCA,2HSC,
     *2HTI,2H V,2HCR,2HMN,2HFE,2HCO,2HNI,2HCD,2HZN,2HGA,2HGE,2HAS,2HSE,
     *2HBR,2HKR,2HRB,2HSR,2H Y,2HZR,2HNB,2HMO,2HTC,2HRU,2HRH,2HPD,2HAG,
     *2HCD,2HIN,2HSN,2HSB,2HTE,2H I,2HXE,2HCS,2HBA,2HLA,2HCE,2HPR,2HND,
     *2HPM,2HSM,2HEU,2HGD,2HTB,2HDY,2HHO,2HER,2HTM,2HYB,2HLU,2HHF,2HTA,
     *2H W,2HRE,2HOS,2HIR,2HPT,2HAU,2HHG,2HTL,2HPB,2HBI,2HPO,2HAT,2HRN,
     *2HFR,2HRA,2HAC,2HTH,2HPA,2H U,2HNP,2HPU,2HAM,2HCM,2HBK,2HCF,
     *2H  ,2H  /
      DATA DFAC/597.7,150.5,86.83,66.85,55.73,50.16,43.02,37.66,31.71,
     *29.85,26.21,24.78,22.33,21.45,19.45,18.79,16.99,15.08,15.41,15.03,
     *13.4,12.58,11.83,11.59,10.97,10.79,10.22,10.26,9.482,9.217,8.642,
     *8.3,8.042,7.63,7.54,7.19,7.049,6.876,6.777,6.605,6.485,6.28,6.086,
     *5.961,5.855,5.663,5.585,5.36,5.247,5.076,4.949,4.722,4.748,4.589,
     *4.533,4.387,4.337,4.3,4.276,4.177,4.099,4.007,3.965,3.831,3.791,
     *3.708,3.653,3.602,3.567,3.482,3.443,3.376,3.33,3.272,3.236,3.168,
     *3.135,3.088,3.059,3.004,2.948,2.908,2.883,2.869,2.869,2.714,2.702,
     *2.666,2.654,2.597,2.608,2.531,.0,.0,.0,.0,.0,.0,.0,.0/
      DATA(ARA(I),I=1,190)/
     $          1.44,.45,.2426,12.0,115.9,1.397,.45,.4845,5.873,52.25,
     $1.6,.45,.7256,3.013,45.78,2.59,.45,.955,.1538,34.75,
     $2.815,.45,1.206,1.060,28.55,2.989,.45,1.445,.9572,28.19,
     $3.35,.45,1.683,1.90,25.13,3.0,.45,1.92,2.0,22.3,
     $2.352,.45,2.157,2.634,18.16,2.199,.45,2.393,2.699,15.68,
     $2.869,.45,2.628,1.854,14.72,4.293,.45,2.862,1.009,13.97,
     $4.739,.45,2.766,.1645,20.23,4.7,.45,3.329,.55,13.21,
     $3.647,.45,3.561,1.56,12.67,3.691,.45,3.792,1.219,12.11,
     $5.714,.45,4.023,.8786,11.78,6.5,.45,4.253,.53,11.23,
     $5.833,.45,4.482,.5457,11.29,6.252,.45,4.71,.5533,11.12,
     $5.884,.45,4.938,.5609,9.995,5.496,.45,5.165,.5685,9.474,
     $5.055,.45,5.391,.9523,9.117,4.489,.45,5.616,1.336,8.413,
     $3.907,.45,5.725,1.461,8.829,3.963,.45,6.065,1.243,7.782,
     $3.535,.45,6.288,1.372,7.361,4.004,.45,6.205,.5551,8.763,
     $4.175,.45,4.673,.3878,21.88,4.75,.45,6.953,.2952,6.809,
     $5.697,.45,7.173,.2026,6.725,6.3,.45,6.496,.11,9.689,
     $6.012,.45,7.611,.2925,6.447,6.656,.45,7.395,.1175,7.684,
     $6.335,.45,8.046,.3652,6.244,7.25,.45,8.262,.22,6.087,
     $6.429,.45,8.478,.2929,6.087,7.159,.45,8.693,.3303,6.003/
      DATA(ARA(I),I=191,380)/
     $7.234,.45,8.907,.3678,5.889,7.603,.45,9.12,.4052,5.765,
     $7.791,.45,9.333,.4427,5.587,7.248,.45,9.545,.4802,5.367,
```

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$7.671,.45,9.756,.5176,5.315,6.887,.45,9.966,.5551,5.151,
$6.677,.45,10.18,.5925,4.919,5.9,.45,10.38,.63,4.758,
$6.354,.45,7.160,.3376,13.94,6.554,.45,10.8,.3555,4.626,
$7.024,.45,11.01,.3709,4.54,7.227,.45,11.21,.3864,4.474,
$8.48,.45,8,608,.348,9.074,7.871,.45,11.62,.3924,4.402,
$8.716,.45,11.83,.3948,4.376,9.289,.45,12.03,.3973,4.384,
$8.218,.45,12.23,.3997,4.447,8.911,.45,12.43,.4021,4.511,
$9.071,.45,12.63,.4045,4.54,8.444,.45,12.83,.4069,4.42,
$8.219,.45,13.03,.4093,4.298,8,.,45,13.23,.4118,4.182,
$7.786,.45,13.43,.4142,4.058,7.58,.45,13.62,.4166,3.976,
$7.38,.45,13.82,.419,3.877,7.591,.45,14,02,.4214,3.863,
$6.996,.45,14.21,.4239,3.725,6.21,.45,14.4,.4263,3.632,
$5.874,.45,14.6,.4287,3.498,5.706,.45,14.79,.433,3.467,
$5.542,.45,14.98,.4335,3.342,5.386,.45,15.17,.4359,3.292,
$5.505,.45,15.36,.4384,3.243,5.657,.45,15.55,.4408,3.195,
$5.329,.45,15.74,.4432,3.186,5.144,.45,15.93,.4424,3.144,
$5.851,.45,16.12,.4416,3.122,5.704,.45,16.3,.4409,3.082/
 DATA(ARA(I),I=381,590)/
$5.563,.45,16.49,.4401,2.965,5.034,.45,16,67,.4393,2.871,
$5.46,.45,18.32,.4385,2.542,4.843,.45,17.04,.4878,2.882,
$5.311,.45,17.22,.537,2.913,5.982,.45,17.4,.5863,2.871,
$6.7,.45,17.8,.677,2.66,6.928,.45,17.77,.5863,2.812,
$6.979,.45,17.95,.5863,2.776,6.954,.45,18.12,.5863,2.748,
$7.82,.45,18.3,.5863,2.737,8.448,.45,18.48,.5863,2.727,
$8.609,.45,18.66,.5863,2.697,8.679,.45,18.83,.5863,2.641,
$8.336,.45,19.01,.5863,2.603,8.204,.45,19.18,.5863,2.573,
$0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
$0,0,0,0,0,0,0,0,0,0,
$.9661,.4126,6.92,8.831,2.582,2.027,.2931,26.34,6.66,.3409,
$1.42,.49,12.25,32.9,161.,2.206,.51,15.32,.25,8.995,
$3.691,.4128,18.48,50.72,9.,4.232,.3877,22.99,35.,7.993,
$2.51,.4752,38.26,13.02,1.892,1.766,.5261,37.11,15.24,2.804,
$1.533,.531,40.44,18.41,2.718,1.183,.55,39.83,17.49,4.001,
$9.894,.3081,23.65,.384,92.93,4.3,.47,34.3,3.3,12.74,
$2.5,.625,45.7,.1,4.359,2.1,.65,49.34,1.788,4.133,
$1.729,.6562,53.41,2.405,3.845,1.402,.5791,58.98,3.528,3.211,
$1.117,.7044,69.69,3.705,2.156,.9172,.724,79.44,3.648,1.646/
 DATA(ARA(I),I=591,780)/
$8.554,.3817,83.61,11.84,1.875,6.297,.4622,65.39,10.14,5.036,
$5.307,.4918,61.74,12.4,6.665,4.71,.5087,65.28,8.806,5.948,
$6.151,.4524,83.,18.31,2.71,6.57,.4322,84.76,15.53,2.779,
$5.738,.4492,84.61,14.18,3.101,5.013,.4707,85.58,16.55,3.211,
$4.32,.4947,76.14,10.85,5.441,4.652,.4571,80.73,22.,4.952,
$3.114,.5236,76.67,7.62,6.385,3.114,.5236,76.67,7.62,7.502,
$3.114,.5236,76.67,7.62,8.514,5.746,.4662,79.24,1.185,7.993,
$2.792,.6346,106.1,.2986,2.331,4.667,.5095,124.3,2.102,1.667,
$2.44,.6346,105.,.83,2.851,1.491,.7118,120.6,1.101,1.877,
$11.72,.3826,102.8,9.231,4.371,7.126,.4804,119.3,5.784,2.454,
$11.61,.3955,146.7,7.031,1.423,10.99,.41,163.9,7.1,1.052,
$9.241,.4275,163.1,7.954,1.102,9.276,.418,157.1,8.038,1.29,
$3.999,.6152,97.6,1.297,5.792,4.306,.5558,97.99,5.514,5.754,
$3.615,.6197,86.26,.333,8.689,5.8,.49,147.2,6.903,1.289,
$5.6,.49,130.,10.,2.844,3.55,.6068,124.7,1.112,3.119,
$3.6,.62,105.8,.1692,6.026,5.4,.53,103.1,3.931,7.767,
$3.97,.6459,131.8,.2233,2.723,3.65,.64,126.8,.6834,3.411,
$3.118,.6519,164.9,1.208,1.51,2.031,.7181,153.1,1.362,1.958,
$14.4,.3923,152.5,8.354,2.597,10.99,.4599,138.4,4.811,3.726/
```

```
      DATA(ARA(I),I=781,880)/
     $16.6,.3773,224.1,6.28,.9121,10.54,.4533,159.3,4.832,2.529,
     $10.33,.4502,162.,5.132,2.444,10.15,.4471,165.6,5.378,2.328,
     $9.976,.4439,168.,5.721,2.258,9.804,.4408,176.2,5.675,1.997,
     $14.22,.363,228.4,7.024,1.016,9.952,.4318,233.5,5.065,.9244,
     $9.272,.4345,210.,4.911,1.258,10.13,.4146,225.7,5.525,1.055,
     $8.949,.4304,213.3,5.071,1.221,11.94,.3783,247.2,6.655,.849,
     $8.472,.4405,195.5,4.051,1.604,8.301,.4399,203.7,3.667,1.459,
     $6.567,.4858,193.,2.65,1.66,5.951,.5015,196.1,2.662,1.589,
     $7.495,.4523,251.4,3.433,.8619,6.335,.4825,255.1,2.834,.8228,
     $4.314,.5558,214.8,2.354,1.263,4.02,.5591,219.9,2.402,1.191/
      DATA(ARA(I),I=881,1000)/
     $3.836,.5765,210.2,2.742,1.305,4.68,.5247,244.7,2.749,.8962,
     $3.223,.5883,232.7,2.954,1.05,2.892,.6204,208.6,2.415,1.416,
     $4.728,.5522,217.,3.091,1.386,6.18,.52,170.,4.,3.224,
     $9.,.47,198.,3.8,2.032,2.324,.6997,216.,1.599,1.399,
     $1.961,.7286,223.,1.621,1.296,1.75,.7427,350.1,.9789,.5507,
     $10.31,.4613,261.2,4.738,.9899,7.962,.519,235.7,4.347,1.313,
     $6.227,.5645,231.9,3.961,1.379,5.246,.5947,228.6,4.027,1.432,
     $5.408,.5811,235.7,3.961,1.358,5.218,.5828,245.,3.838,1.25,
     $0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
     $0,0,0,0,0,0,0,0,0,0/
       DATA ATMASS/1.008,4.003,6.939,9.012,10.811,12.011,14.007,15.999,
     A 18.998,20.183,22.989,24.312,26.982,28.086,30.974,32.064,35.453,
     B 39.948,39.102,40.08,44.956,47.90,50.942,51.996,54.9380,55.847,
     C 58.933,58.71,63.511,65.37,69.72,72.59,74.922,78.96,79.909,83.80,
     D 85.47,87.62,88.905,91.22,92.906,95.94,99.00,101.07,102.905,
     E 106.40,107.870,112.40,114.82,118.69,121.75,127.60,126.904,
     F 131.30,132.905,137.34,138.91,140.12,140.907,144.24,
     G 145.0,150,35,151.96,157.25,158.924,162.50,164.930,167.26,
     H 168.934,173.04,174.97,178.49,180.94,183.85,186.2,190.2,192.2,
     I 195.09,196.967,200.59,204.37,207.19,208.980,242.0,210.0,
     J 222.0,223.0,227.0,227.0,232.038,231.0,238.03,237.0,242.0,
     K 243.0,245.0,249.0,249.0,254.0,252.0/
      DATA EREF/0.01,0.02,0.03,0.04,0.05,0.06,0.07,0.08,0.09,0.1,0.15,
     *0.2,0.25,0.3,0.35,0.4,0.45,0.5,0.55,0.6,0.65,0.7,0.75,0.8,0.85,
     *0.9,0.95,1.,2.,3.,4.,5.,6.,7.,8.,9.,10./
11    FORMAT(I8,F14.2,3X,5(7X,A2,F10.2,1X))
600   FORMAT(10I5)
101   FORMAT(1H1,45X,26HENERGY LOSS REFERENCE DATA//
     *30X,10HPARTICLE 1,55X,10HPARTICLE 2/
     *32X,A2,1H-,I3,59X,A2,1H-,I3//
     *5X,6HTARGET,5(5X,A2))
102   FORMAT(1H+,75X,5(5X,A2))
103   FORMAT(3X,7HMEV/AMU,58X,7HMEV/AMU)
104   FORMAT(1X,F9.3,3X,5F7.3)
105   FORMAT(1H+,65X,F9.3,3X,5F7.3)
106   FORMAT(1X,F9.3,3X,15F7.3)
111   FORMAT(1H1,45X,33HENERGY LOSS VALUES FOR THE TARGET//
     *52X,17HINCOMING PARTICLE/57X,A2,1H-,I3//6X,5HLAYER,15I7)
112   FORMAT(1H1,45X,33HENERGY LOSS VALUES FOR THE TARGET//
     *52X,17HOUTGOING PARTICLE/57X,A2,1H-,I3//6X,5HLAYER,15I7)
113   FORMAT(4X,6HENERGY)
      M=1
      DO 300 J=1,2
      DO 300 I=1,100
      DO 300 K=1,5
```

```
      ACO(K,I,J)=ARA(M)
      M=M+1
  300 CONTINUE
      READ(5,600)ZIN(1),ZIN(2)
C      ICON=0 IMPLIES THAT NO CONCEN-TABLE NECC. OTHERWISE YES.
      READ(5,600)IZA,(ZTARG(K),K=1,5),ICON
C
      DO 1000 I=1,5
      DO 1000 J=1,NLAYER
      CATARG(I,J)=0.$ATARG(I,J)=0.$DUMT(J)=0.
 1000 CONTINUE
      JZ=IZA-1
      DO 602 I=1,JZ
      READ(5,*)(ATARG(I,K),K=1,NLAYER)
      DO 602 J=1,NLAYER
      DUMT(J)=DUMT(J)+ATARG(I,J)
  602 CATARG(I,J)=ATARG(I,J)
      DO 100 I=1,NLAYER
      ATARG(IZA,I)=100.-DUMT(I)
      CATARG(IZA,I)=ATARG(IZA,I)
C     PROVISION IS MADE FOR 5 CONSTITUENTS IN EACH LAYER.
      ATSUM=0.
C          ZTARG IS THE ATOMIC NUMBER OF EACH CONSTITUENT.
C     ATARG IS THE ATOMIC PERCENTAGE OF EACH CONSTITUENT.
C     THE SUM OF THE ATARGS MUST BE EXACTLY 100.
C       REL CONCEN IS CALCULATED IN HERE.
        DO 500 IAT=1,5
        IF(ZTARG(IAT).EQ.0.)GO TO 500
        AMA=ATMASS(ZTARG(IAT))
        IF(AMA.EQ.0.)GO TO 500
      ATSUM=ATSUM+AMA*ATARG(IAT,I)
  500   CONTINUE
        IF(ATSUM.EQ.0.)GO TO 501
        DO 506 IAZ=1,5
  506 CONCEN(IAZ,I)=ATARG(IAZ,I)/ATSUM
        GO TO 502
  501    DO 511 IAZ=1,5
  511    CONCEN(IAZ,I)=1.
  502   CONTINUE
        DO 505 IAT=1,5
        IF(ZTARG(IAT).EQ.0.)GO TO 505
      ATARG(IAT,I)=ATARG(IAT,I)*ATMASS(ZTARG(IAT))
  505   CONTINUE
      FACTOR=ATARG(1,I)+ATARG(2,I)+ATARG(3,I)+ATARG(4,I)+ATARG(5,I)
      IF(FACTOR.LT.0.9) GO TO 100
      CALL SETION(ZTARG,FION(I),I)
      DO 15 K=1,5
      IF(ZTARG(K).LT.1.OR.ZTARG(K).GT.100) ZTARG(K)=100
   15 CONTINUE
      IF(ISSW(8).NE.1)GO TO 3004
      WRITE(6,11)I,FION(I),(SYMB(ZTARG(K)),CATARG(K,I),K=1,5)
 3004 CONTINUE
  100 CONTINUE
      IF(ISSW(1).NE.1)GO TO 200
C     OUTPUT ENERGY LOSS DATA FOR THE INDIVIDUAL TARGET CONSTITUENTS
      MASS1=IFIX(M1+.5)
      MASS2=IFIX(M3+.5)
```

```
      WRITE(6,101)SYMB(ZIN(1)),MASS1,SYMB(ZIN(2)),MASS2,(SYMB(ZTARG(I)),
     *I=1,IZA)
      WRITE(6,102)(SYMB(ZTARG(I)),I=1,IZA)
      WRITE(6,103)
      DO 110 I=1,37
      DO 155 J=1,2
      IP=ZIN(J)
      PI=ATMASS(1)
      IF(IP.EQ.2)PI=ATMASS(2)
      F=EREF(I)*PI/M1
      IF(J.EQ.2)E=EREF(I)*PI/M3
      DO 154 K=1,IZA
      JP=ZTARG(K)
      A1=ACO(1,JP,IP)
      A2=ACO(2,JP,IP)
      A3=ACO(3,JP,IP)
      A4=ACO(4,JP,IP)
      A5=ACO(5,JP,IP)
      SFAC=DFAC(JP)*.001
      SL=A1*(E*1000.)**A2
      SH=A3*ALOG(1.+A4/E+A5*E)/E
  154 S1(K,I,J)=SL*SH/(SL+SH)*SFAC
      IF(J.EQ.2)GO TO 155
      WRITE(6,104)E,(S1(K,I,1),K=1,IZA)
  155 CONTINUE
      WRITE(6,105)E,(S1(K,I,2),K=1,IZA)
  110 CONTINUE
C
C     OUTPUT THE ENERGY LOSS VALUES FOR THE FIRST 15 LAYERS
      NZ=NLAYER
      IF(NLAYER.GT.15)NZ=15
      DO 125 M=1,2
      IF(M.EQ.2)GO TO 127
      WRITE(6,111)SYMB(ZIN(1)),MASS1,(N,N=1,NZ)
      GO TO 126
  127 WRITE(6,112)SYMB(ZIN(2)),MASS2,(N,N=1,NZ)
  126 WRITE(6,113)
      IP=ZIN(M)
      PI=ATMASS(1)
      IF(IP.EQ.2)PI=ATMASS(2)
      DO 121 I=1,37
      E=EREF(I)*M1/PI
      IF(M.EQ.2)E=EREF(I)*M3/PI
      DO 120 J=1,NZ
      S2(J)=0.
      DO 120 K=1,IZA
  120 S2(J)=S2(J)+S1(K,I,M)*CATARG(K,J)/100.
      WRITE(6,106)E,(S2(N),N=1,NZ)
  121 CONTINUE
  125 CONTINUE
  200 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE WIDTH(E,DE,M,I,WID,L)
C     THIS SUBROUTINE CALCULATES THE STANDARD DEVIATION OF THE ENERGY
C        LOSS STRAGGLING.
C     THE EXPRESSION FOR ENERGY LOSS STRAGGLING, WID, IS FROM THE
C        BOHR MODEL AS DESCRIBED BY DEARNALEY AND NORTHROP, 'SEMICON-
C        DUCTOR COUNTERS FOR NUCLEAR RADIATION', 1963.  THE SAME EXPRE-
C        SSION IS FOUND IN CHU, MAYER,AND NICOLET,'BACKSCATTERING
C        SPECTROMETRY', 1978.  THE LINDHARD AND SCHARFF'S CORRECTION
C        FACTOR FOR LOW AND MEDIUM ENERGY PROJECTILES IS USED.
C        E - PROJECTILE ENERGY IN MEV
C        DE - ENERGY LOSS IN MEV
C        M - PROJECTILE MASS
C        I - IONIZATION POTENTIAL OF THE LAYER IN EV.  CALCULATED IN
C           SETION.
C        WMAX - MAXIMUM ENERGY TRANSFERRED TO AN ELECTRON IN EV.
C        WID - STANDARD DEVIATION OF THE ENERYY LOSS STRAGGLING
C           DISTRIBUTION.
      REAL I,M
      COMMON/FLAGS/FLAG,FLAGA,FLAGB,FLAGC,FLAGD,FLAGE
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      COMMON/TABLES/ACO(5,100,2),CONCEN(5,100),CATARG(5,100),DFAC(100)
      COMMON/S/VALUE(2000),ISSW(10)
      IF(ISSW(2).NE.1)GO TO 20
      IF(DE.LT.1.E-10)GO TO 20
      WMAX=4.*E/M*5.486E+2
      Z2=0.
      DO 1 J=1,5
    1 Z2=Z2+ZTARG(J)*CATARG(J,L)/100.
      CHI=39.5839*E/(M*Z2)
      CLO=ALOG(WMAX/I)
      IF(CHI-3.)2,2,3
    2 WID=SQRT((WMAX*DE*1.E-6)/4.)
      RETURN
    3 IF(CLO.LE.0.)GO TO 10
      WID=SQRT(WMAX/(2.*DE*1.E6*CLO))*DE
      RETURN
   10 FLAGC=1.
   20 WID=0.
      RETURN
      END
```

```
      SUBROUTINE PICKE(F,E0,SIG,E)
C
C     THIS SUBROUTINE FINDS THE VALUE OF E SUCH THAT THE INTEGRAL
C          OF THE GAUSSIAN DISTRIBUTION FROM MINUS INFINITY
C          TO E EQUALS F.  THE INTEGRAL FOR ALL E GIVES F = 1.00
C
      FA=F-0.5
      E=E0
C     FA IS THE AREA BETWEEN E AND E0.
      IF(FA)10,100,20
C     F LESS THAN 0.5
   10 FA=0.5-F
      CALL FINDE(FA,X)
      X=-X
      GO TO 30
C     F GREATER THAN 0.5
   20 CALL FINDE(FA,X)
   30 E=E0+X*SIG
  100 CONTINUE
      RETURN
      END



      SUBROUTINE FINDE(F,X)
C
C     X IS FOUND SUCH THAT INTEGRAL FROM 0 TO X IS F.
C     X=(E-E0)/SIG
C
      IF(F.LT.0.04) GO TO 10
C     Q IS THE INTEGRAL FROM X TO INFINITY
      Q=0.5-F
       IF(Q.LT.1.E-10) Q=1.E-10
C     THIS EXPRESSION IS FROM HASTINGS, 'APPROXIMATIONS FOR DIGITAL
C     COMPUTERS', SHEET 68.
      U=SQRT(ALOG(1./Q**2))
      X=U-(2.515517+U*(0.802853+U*0.010328))/
     * (1.+U*(1.432788+U*(0.189269+U*0.001308)))
      RETURN
   10 X=F/0.3989423
      RETURN
      END
```

```
      SUBROUTINE DIST(E,SIG,WT,EMAX,EMIN)
C
C     THIS ROUTINE DISTRIBUTES A GAUSSIAN INTO 'VALUE' GIVEN THE
C          MEAN VALUE(E), AND THE STANDARD DEVIATION (SIG).
C
C     VALUE CONTAINS 2000 BINS.
C     WT IS USED TO WEIGHT THE ENTIRE DISTRIBUTION.
C     EMIN AND EMAX DEFINE THE ENERGY SPAN OF VALUE.
C
      COMMON/S/VALUE(2000),ISSW(10)
      FACTOR=2000./(EMAX-EMIN)
      EA=EMIN-E
C     LIMIT THE GAUSSIAN TO FIVE STANDARD DEVIATIONS.
      EL=E-5.*SIG
      NL= (EL-EMIN)*FACTOR
      IF(NL.LT.1) NL=1
      EH=E+5.*SIG
      NH= (EH-EMIN)*FACTOR
      IF(NH.GT.2000) NH=2000
      SIGA=1./(SIG*1.4142)
      ACON=SIGA*EA
      AX=SIGA/FACTOR
      TH= AX*(NL-1)+ACON
      CALL IGAUS(TH,UH)
      DO 100 I=NL,NH
      TH=AX*I+ACON
      UL=UH
      CALL IGAUS(TH,UH)
  100 VALUE(I)=VALUE(I)+(UH-UL)*WT
      RETURN
      END



       SUBROUTINE IGAUS(T,F)
C
C     FIND F8 THE AREA BENEATHE THE GAUSSIANB FROM - INFIN TO T
C     T=(E-E0)*SQRT(0.5)/SIG
C     THE AREA FOR ALL T IS 1.0
C
      V=ABS(T)
      C1=0.0705230784
      C2=0.0422820123
      C3= 0.0092705272
      C4= 0.0001520143
      C6= 0.0002765672
      C5= 0.0000430638
      U=0.5/(1.+V*(C1+V*(C2+V*(C3+V*(C4+V*(C5+V*C5))))))**16.
C     U IS THE INTEGRAL FROM - INFIN TO -V  TAKEN FROM NBS-AMS-55.
C      ERROR IS LT 1.E-7
      F=U
      IF(T.GT.0.)F=1.-U
      RETURN
      END
```

```
      SUBROUTINE KIN(E,ANGL,E3,XSEC,KM)
C
C     THIS IS A CLASSICAL KINETICS SUBROUTINE.  XSEC IS LABORATORY.
C     THE REACTION IS M1(M2,M3)M4.
C
      REAL M1,M2,M3,M4
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      COMMON /FLAGS/FLAG,FLAGA,FLAGB,FLAGC,FLAGD,FLAGE
      D=(M1+M2)*(M3+M4)
      C=E/(D*(E+Q))
      A=M1*M4*C
      B=M1*M3*C
      E3=1.0+M1*Q/(M2*(E+Q))
      C=M2*E3/D
      D=C*M4
      C=C*M3
C     SET FLAG=1 IF DOUBLE VALUED
      IF(B.GT.D) FLAG=1.0
      XSEC=0.
      E3=0.
      U=D/B-SIN(ANGL)**2
      IF(U.LT.0.) RETURN
      U=SQRT(U)
      E3=(E+Q)*B*(COS(ANGL)+U)**2
      V=(E3/(E+Q)-B-D)/(2.*SQRT(A*C))
      IF(V.GT.0.7) GO TO 10
      IF(V.LT.-0.7) GO TO 20
      ANGCM=ACOS(V)
      GO TO 30
   10 ANGCM=ASIN(SQRT(E3/(E+Q)/D)*SIN(ANGL))
      GO TO 30
   20 ANGCM=3.141592654-ASIN(SQRT(E3/(E+Q)/D)*SIN(ANGL))
C     GET CENTER OF MASS CROSS-SECTION.
30      CALL SIG(E,ANGCM,XSEC,KM)
C     CONVERT TO LABORATORY CROSS-SECTION.
      XSEC=XSEC*E3/(SQRT(A*C)*U*(E+Q))
      RETURN
      END
```

```
      SUBROUTINE SIG(E,ANGCM,XSEC,KM)
C       THIS SUBROUTINE CALCULATES THE REACTION XSEC FOR
C      M1(M2,M3)M4 RUTHERFORD IF M2=56 , FOR O(D,P1) IF M2=16, AND FOR
C      N(D,P5) FOR M2=14.
C      FOR C(D,P0) FOR M2=12.
       REAL M1,M2,M3,M4
           COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
       DIMENSION EN(40),XO(40),XN(40),XC(40)
          INTEGER ZIN,ZTARG
         DATA (EN(I),I=1,40)/.3,.31,.32,.33,.34,.35,.36,.37,.38,.39,.40,
     $.41,.42,.43,.44,.45,.46,.47,.48,.49,.50,.51,.52,.53,.54,.55,.56,
     $.57,.58,.59,.60,.61,.62,.63,.64,.65,.66,.67,.68,.69/
       DATA(XO(I),I=1,40)/0.,.01,.025,.03,.035,.04,.046,.055,.066,.082,
     $.10,.129,.160,.200,.235,.270,.310,.350,.390,.440,.500,.580,.690,
     $.800,.930,1.050,1.210,1.380,1.510,1.640,1.720,1.785,1.835,1.875,
     $1.900,1.920,1.940,1.955,1.965,1.970/
       DATA(XC(I),I=1,40)/0.208,0.209,0.210,0.211,0.215,0.219,0.220,0.22,
     $0.224,0.225,0.229,0.230,0.231,0.240,0.249,0.251,0.261,0.271,
     $0.288,0.305,0.324,0.340,0.360,0.385,0.411,0.445,0.480,0.520,0.560,
     $0.610,0.660,0.715,0.772,0.840,0.915,0.999,1.100,1.250,1.430,1.610/
       DATA(XN(I),I=1,40)/.015,.020,.024,.028,.037,.047,.058,.074,.092,.1
     *14,.139,.169,.202,.235,.279,.318,.368,.423,.478,.539,.599,.660,.72
     *7,.793,.849,.905,.939,.961,.951,.929,.897,.886,.887,.898,.954,1.02
     *7,1.111,1.190,1.268,1.369/
          Z1=ZIN(1)
          Z2=ZTARG(KM)
C          IF Q.EQ.0. ELASTIC SCATTERING
          IF(Q.EQ.0.)GO TO 10
       CM2=M2-16.
       CM2=ABS(CM2)
       ICM=1
       IF(CM2.LT.1.0)GO TO 20
       CM3=M2-14.
       CM3=ABS(CM3)
       ICM=2
       IF(CM3.LT.1.0)GO TO 20
       CM4=M2-12.
       CM4=ABS(CM4)
       ICM=3
       IF(CM4.LT.1.0)GO TO 20
C      THIS SECTION CALCULATES THE RUTHERFORD CROSS SECTION OF THE
C         REACTION M2(M1,M3)M4
 10    CS=1./SIN(ANGCM/2.)
       CS4=CS**4
          XSEC=1.296*(Z1*Z2/E)**2 *((M1+M2)/M2)**2*CS4
       RETURN
 20    IF(E.LT.EN(1).OR.E.GT.EN(40))GO TO 100
       DO 21 I=1,39
       EHI=EN(I+1)
       ELO=EN(I)
       IF(E.GE.ELO.AND.E.LE.EHI)GO TO 22
 21    CONTINUE
 22    CONTINUE
       DEE=EHI-ELO
       DE=E-ELO
       IF(ICM-2)23,24,25
```

```
C       THIS SECTION CALCULATES THE O(D,P1) CROSS SECTION FROM
C       DATA TABLE FIG9  CROSS SECTION VALUES ARE FROM LONGEQUE ET.AL..
C       JOURNAL DE PHYSIQUE84UNE 65. THEY ARE GOOD ONLY FOR 160 DEGR LAB
C       ANGLE
23        XSEC=XO(I)+(XO(I+1)-XO(I))*DE/DEE
        RETURN
C       CROSS SECTION.VALUES ARE EXTRAPOLATED FROM THE DATA OF NIILER AND
C       BIRKMIRE(REF TO BOOTH ET.AL. (PROC PHYS SOC.711(1957),325.)
24      XSEC=XN(I)+(XN(I+1)-XN(I))*DE/DEE
        RETURN
C       THIS SECTION CALCULATES THE C(D,P0) CROSS SECTION AND IT IS GOOD
C       FOR 160 DEGR LAB ANGLE
C        C(D,P0) HUEZ ETAL, NIM 105(1972)197
25      XSEC=XC(I)+(XC(I+1)-XC(I))*DE/DEE
        RETURN
C       ENERGY OUT OF RANGE OF TABLE INPUT
100     XSEC=0.
        RETURN
C       MASS OF TARGET IS WRONGBRESTART PROGRAM
        END
```

```
      SUBROUTINE SHAPE (E,DE,WID,FMASS,ION,FION,THICK,THKVAR,LAYER)
C
C     THIS SUBROUTINE CALCULATES THE MEAN ENERGY AND STANDARD DEVIATION
C         AS PARTICLES TRAVERSE ALL BUT THE FINAL LAYER.
C
C     E IS THE INITIAL PARTICLE ENERGY.
C     FMASS IS THE PARTICLE MASS.
C     THICK IS THE ARRAY OF LAYER THICKNESSES.
C     FION IS THE ARRAY OF IONIZATION POTENTIALS.
C     LAYER IS THE NUMBER OF THE DESIRED LAYER.
C     ION IS THE ID FOR THE PARTICLE, 1 IS BEAM AND 2 IS OUTGOING.
C
        COMMON/SHA/NSLA(100),WT(100)
      DIMENSION THICK(1),FION(1),THKVAR(1)
C     CUTOFF SET AT 1 KEV
      IF(E.LT.1.E-3) GO TO 20
      WID=0.
      DE=WID2=0.0
      IF(LAYER.LE.1) RETURN
      EA=E
      NLAY=LAYER-1
      IF(LAYER.GT.2.AND.THKVAR(1).NE.0.AND.ION.EQ.2)NLAY=LAYER-2
      DO 10 I=1,NLAY
      II=I
      IF(ION.EQ.2) II=LAYER-I
      IF(THICK(II).LE.0.0) GO TO 10
        UA=1.
      NSLAB=NSLA(II)
      THKN=THICK(II)/NSLAB
      DO 30 J=1,NSLAB
   31 THKA=THKN*UA
      CALL ELOSS(EA,II,ION,THKA,DE)
      IF(EA.LT.DE) GO TO 20
      CALL WIDTH(EA,DE,FMASS,FION(II),WID,LAYER)
      WID2=WID2+WID**2
      EA=EA-DE
   30 CONTINUE
      DE=E-EA
   10 CONTINUE
      WID=SQRT(WID2)
      RETURN
C     EITHER DE CANNOT BE FOUND OR PARTICLE IS STOPPED
C          IN EITHER CASE, PARTICLE IS ASSUMED STOPPED
C     DE GREATER THAN E IS USED TO FLAG THE CALLING PROGRAM.
   20 DE=E+E
      WID=0.0
      RETURN
      END
```

```
      SUBROUTINE ELOSS(E,LAY,ION,T,DE)
C     THIS ROUTINE CALCULATES THE ENERGY LOSS OF PROTONS, DEUTERONS,
C        TRITONS , ALPHAS OR HE3'S AT THE ENERGY E (MEV).  M1 AND ZIN(1)
C        ARE THE MASS AND CHARGE OF THE INCIDENT PARTICLE, M3 AND ZIN(2)
C        ARE THE MASS AND CHARGE OF THE OUTGOING PARTICLE.  ZTARG(I)
C        GIVES THE CHARGE OF THE I'TH TARGET CONSTITUENT, CATARG(I,J)
C        GIVES THE ATOMIC PERCENT OF THE I'TH CONSTITUENT IN THE J'TH
C        LAYER.  T IS THE SLAB THICKNESS.  THE EXPRESSION FOR DE IS FROM
C        A/Z.  FOR ALPHAS, IT IS GOOD  10 TO 10,000 KEV AND FOR PROTONS,
C        GOOD FROM 10 TO 1000 KEV.  FOR PROTONS, IF USED AT 10 MEV, THE
C        ERROR IS LESS THAN 5 PERCENT.
      COMMON/TABLES/ACO(5,100,2),CONCEN(5,100),CATARG(5,100),DFAC(100)
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      COMMON/ELO/IZA
      REAL M1,M2,M3,M4
      INTEGER ZIN,ZTARG
      IF(E.EQ.0.)GO TO 11
      IP=ZIN(ION)
      DE=0.
      PI=1.008
      IF(IP.EQ.2)PI=4.003
      EC=E*PI/M1
      IF(ION.EQ.2)EC=E*PI/M3
      DO 10 J=1,IZA
      JP=ZTARG(J)
      IF(JP.EQ.0)GO TO 10
      A1=ACO(1,JP,IP)
      A2=ACO(2,JP,IP)
      A3=ACO(3,JP,IP)
      A4=ACO(4,JP,IP)
      A5=ACO(5,JP,IP)
      SFAC=DFAC(JP)*0.001
      SL=A1*(EC*1000.)**A2
      SH=A3*ALOG(1.+A4/EC+A5*EC)/EC
      DE=DE+CATARG(J,LAY)*SL*SH*SFAC/(100.*(SL+SH))
10    CONTINUE
      DE=DE*T
11    EL=.01
      EH=10.0
      IF(EC.LT.EL.OR.EC.GT.EH)WRITE(6,1)EC
1     FORMAT(4X,6HENERGY,F10.4,46HMEV. OUT OF RANGE OF ANALYTICAL A/Z EX
     *PRESSION)
      RETURN
      END
```

```
      SUBROUTINE OUTPUT(YMAX2)
C
C     THIS ROUTINE PREPARES THE CALCULATED AND EXPERIMENTAL DISTRI-
C        BUTIONS FOR PLOTTING. IT DOES LEAST SQUAREO FITTING OF THE TWO.
C
          COMMON/OU/X(410),Y(410),YY(410),XX(410)
      COMMON/S/VALUE(2000),ISSW(10)
      COMMON/OEX/EMIN,EMAX
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      REAL M1,M2,M3,M4
      COMMON/PLO/LP(400,125)
      DIMENSION AX(400),AY(400),AYX(400),EXX(400)
C     CONDENSE THE OUTPUT BY A FACTOR OF FIVE.
      DO 1111 I=1,410
      X(I)=0.$Y(I)=0.$YY(I)=0.
1111  CONTINUE
      DELE=(EMAX-EMIN)*5./2000.
      YMAX=0.0
      READ(5,111)XSC,YSFA
      READ(5,111)AY1,AY2,BY1,BY2
      DO 10 I=1,400
          X(I)=I
      J=I*5-4
      Y(I)=VALUE(J)+VALUE(J+1)+VALUE(J+2)+VALUE(J+3)+VALUE(J+4)
  111 FORMAT(4F10.5)
 10   CONTINUE
      IF(ISSW(7).EQ.1)WRITE(6,75)
          DO 151 I=1,400
          XX(I)=X(I)
 151      YY(I)=Y(I)
 15       CONTINUE
C
C     ZERO THE ARRAY USED FOR ACCUMULATING THE DISTRIBUTION.
C
      ENTRY OUT1
      DO 100 I=1,2000
  100 VALUE(I)=0.0
      RETURN
C
C     PLOT THE DATA FOR COMPARISON.
C
      ENTRY OUT2
      READ(5,1000)BIAS,CALX
1000    FORMAT(F8.0,1PE12.5)
C     BIAS IS THE NO OF CHANNELS THE DATA ARE OFFSET FROM ZERO
C     CALX IS THE ENERGY SCALE CALIBRATION IN MEV/CHANNEL
21      FORMAT(10F8.0)
      READ(5,112)ICNT
C     ICNT GIVES THE NUMBER OF DATA POINTS TO BE READ.  ICNT.LE.400
      READ(5,21)(X(I),Y(I),I=1,ICNT)
      SUMXC=SUMX2=0.
      YMAX=0.0
      NPTS=0
      YMAX2=0$IX=0$KSS=0
      DO 20 I=1,ICNT
      EX=(X(I)-BIAS)*CALX
      DO 23 JC=1,400
```

```
      EC=EMIN+DELE*XX(JC)
      IF(EC.GT.EX.AND.EX.GE.EMIN)GO TO 24
   23 CONTINUE
   24 AY(I)=(YY(JC)-YY(JC-1))*(EC-EX)/DELE+YY(JC-1)
      IF(EX.GE.EMIN.AND.IX.EQ.0)IX=I
      IF(EX.GE.AY1.AND.EX.LE.AY2)GO TO 999
      GO TO 998
  999  SUMXC=SUMXC+AY(I)*Y(I)
      SUMX2=SUMX2+Y(I)*Y(I)
  998 CONTINUE
      AX(I)=X(I)
      AYX(I)=Y(I)
      IF(EX.LE.EMAX)NPTS=NPTS+1
   20 CONTINUE
   25 CONTINUE
      ASUM=SUMXC/SUMX2
      NPS=NPTS
      DO 50 J=1,ICNT
      Y(J)=AYX(J)*ASUM
   50 YMAX=AMAX1(YMAX,Y(J),AY(J))
      YSC=YMAX/YSFA
C
C     CALCULATION OF THE XISQ OVER ENERGY REGION AY1 TO AY2
C
      XISQ=0.
      KS=0
   75 FORMAT(1H1)
      NK=0
      DO 980  J=1,ICNT
      AYX2=0 $ AY22=0
      EX=(AX(J)-BIAS)*CALX
      EX1=EX
C
C     CAREFUL***   THE FOLLOWING STATEMENT WITH ITS NUMBERS IS GOOD ONLY
C        FOR C,N,O ANALYSIS AT 670 KEV.
      IF(EX.GT.2.5)EX1=EX-0.75
      AYX(J)=ASUM*AYX(J)/YSC
      AY(J)=AY(J)/YSC
      IF(NK.EQ.1)AYX2=(AYX(J-1)+AYX(J))/2.
      IF(NK.EQ.1)AY22=(AY(J-1)+AY(J))/2.
      NK=NK+1
      IF(NK.EQ.2)NK=0
      IF(ISSW(7).NE.1)GO TO 2000
      IF(EX.GT.EMAX)GO TO 2000
      WRITE(6,112)KS,EX,AYX(J),AY(J),EX1,AYX2,AY22
  112 FORMAT(I5,2(10X,F8.4,2F10.3))
 2000 CONTINUE
      KSS=KSS+1
      EXX(KSS)=EX
      YEX=AYX(J)
      IF(YEX.EQ.0.)YEX=1.
  996 IF(EX.GE.AY1.AND.EX.LE.AY2)GO TO 991
      GO TO 980
  991 XISQ=XISQ+YSC*(AY(J)-AYX(J))**2/(YEX*ASUM)
      KS=KS+1
  980 CONTINUE
      SK=KS $ XISQ=XISQ/SK
```

```
C       PLOT THE EXPERIMENTAL DATA
        WRITE(6,2)CALX,BIAS,YMAX,XISQ,SK,ASUM
2       FORMAT(//18H PLOT EXP/CAL DATA/,2X,25HTHE ENERGY CALIBRATION IS,
       *F10.6,36H   KEV/CH AND THE ZERO LEVEL BIAS IS,F10.2,9H CHANNELS/
       *21H FULL SCALE VALUE IS ,1PE12.5,/20H XISQ PER POINT IS  ,1PE12.5,
       *6H WITH ,0PF10.2,15HPOINTS INCLUDED/12H ASUM IS     ,1PE12.5)
        IF(ISSW(5).NE.1)GO TO 1515
        CALL PLOT1(AYX,AY,EXX,YSC,NPS,IX,KSS,ICNT)
1515    CONTINUE
        RETURN
        END
```

```
      SUBROUTINE PLOT1(AYX,AY,EEX,YSC,NPS,IX,KS,ICNT)
      COMMON/PLO/LP(400,125)
      DIMENSION AYX(1),AY(1),EEX(1)
      DIMENSION IS(4)
      DATA(IS(I),I=1,4)/1H ,1H0,1H.,1H$/
      NPTS=NPS-1
      NPTS=IX+NPTS
      DO 1 I=1,125
      DO 1 J=1,ICNT
1     LP(J,I)=IS(1)
      IXX=IX
      KL=NPS
C
C     THIS  PLOTS THE CALCULATED DATA
C     ****************************************      ************
      DO 5 K= IX,NPTS
      XI=AY(K)
      IXI=XI$XII=IXI$DX=XI-XII$IF(DX.GE.0.5)IXI=IXI+1$J=IXI
      IF(J.LE.0)J=1
      LP(KL,J)=IS(3)
C
C     THIS PLOTS THE EXPERIMENTAL DATA
C
      XI=AYX(K)$IXI=XI$XII=IXI$DX=XI-XII$IF(DX.GE.0.5)IXI=IXI+1$I=IXI
      IF(I.LE.0)I=1
      LP(KL,I)=IS(2)
C
C     ****************************************      ************
      IF(J.EQ.I)LP(KL,I)=IS(4)
      KL=KL-1
      IF(KL.LE.0)KL=1
5     CONTINUE
      KM=1$KL=NPS$N=9
      WRITE(6,29)
29    FORMAT(1H1)
      WRITE(6,31)
31    FORMAT(1H ,50X,13HPROFILE CURVE)
      DO 50 K=1,NPS
       IF(KM.EQ.K.AND.EEX(KM).NE.0)GO TO 40
      WRITE(6,30)(LP(KL,I),I=1,120)
 30   FORMAT(7X,1HI,120A1,1HI)
        KL=KL-1
      IF(KL.EQ.0)KL=1
       GO TO 50
 40   WRITE(6,35)EEX(KM),(LP(KL,I),I=1,120)
 35   FORMAT(1X,F5.2,1X,1HI,120A1,1HI)
      KM=KM+N
      N=10
        KL=KL-1
      IF(KL.EQ.0)KL=1
50    CONTINUE
      WRITE(6,51)
 51   FORMAT(8X,12(10H+---------),2H++)
      WRITE(6,55)
55    FORMAT(1H ,50X,5HYIELD)
       IX=IXX
      RETURN
      END
```

```
      SUBROUTINE SWITCH
      COMMON/S/VALUE(2000),ISSW(10)
C     A SWITCH IS DESIGNATED BY ISSW(I) IN THE PROGRAM.
C     THE SWITCHES ARE BEING USED AS FOLLOWS.
C     1 - OUTPUTS ENERGY LOSS INFORMATION, BOTH FOR TARGET CONSTITUENTS
C        (ELEMENTS) AND COMPOSITE LAYERS.
C     2 - WHEN ON INCLUDES ENERGY LOSS STRAGGLING IN THE CALCULATION
C     3 - OUTPUTS THE PR INFO.  USEFUL THINGS ARE INCIDENT, SCATTERED
C        AND OUTGOING ENERGY AND CROSS SECTIONS.
C        CURRENTLY NO-OP
C     4 - OUTPUTS ALL PERTINENT INFORMATION ON THE RUN BEING DONE -
C        REACTION, GEOMETRIES, ETC.   SHOULD ALWAYS BE ON.
C     5 - GIVES THE PRONTER PLOT OF EXPERIMENTAL AND CALC. SPECTRA
C     6 - OUTPUTS ENERGIES, CROSS SECTIONS AS A FUNCTION OF SLAB.
C        VERY USEFUL WHEN ITERATING CONCENTRATIONS TO FIT DATA.  CAN
C        BE A VERY LONG OUTPUT.
C     7 - OUTPUTS NUMERICAL LIST OF CHANNEL NO. VS EXPERIMENTAL AND
C        CALCULATED YIELDS.
C     8 - OUTPUTS TARGET COMPOSITION DATA.
C     9 - PRINTS THIS SWITCH INFORMATION.
C     10 - OUTPUTS CONCENTRATION TABLE.
      READ (5,2)(ISSW(I),I=1,10)
2     FORMAT(10I1)
      IF(ISSW(9).NE.1)GO TO 5
      WRITE(6,10)
10     FORMAT(1H1)
      WRITE(6,11)
 11   FORMAT(1X,' SWITCH 1 ON FOR ENERGY LOSS INFORMATION'/
     *1X,' SWITCH 2 IS ON FOR ENERGY LOSS STRAGGLING CALCULATION'/
     *1X,' SWITCH 3 ON FOR PUBLIC RELATIONS INFORMATION'/
     *1X,' SWITCH 4 ON FOR PERTINENT DATA ON CURRENT CALCULATION'/
     *1X,' SWITCH 5 ON FOR PRINTER PLOT OF RESULTS'/
     *1X,' SWITCH 6 ON FOR USEFUL DATA WHILE DOING INTERATIONS'/
     *1X,' SWITCH 7 ON FOR NUMERICAL LIST OF PLOTTED RESULTS'/
     *1X,' SWITCH 8 ON FOR TARGET COMPOSITION DATA'/
     *1X,' SWITCH 9 ON FOR SWITCH INFORMATION TABLE'/
     *1X,' SWITCH 10 ON FOR LAYER CONCENTRATION TABLE'/
     *1X,' NORMAL RUNNING SHOULD HAVE SWITCHES 4,5,7,8,10 ON')
 5    RETURN
      END
```

```
      SUBROUTINE CONCTAB(NLAYER,THICK)
      COMMON/TABLES/ACO(5,100,2),CONCEN(5,100),CATARG(5,100),DFAC(100)
      COMMON/TSYMB/SYMB(100),ICON
      COMMON/REACT/M1,M2,M3,M4,Q,ZIN(2),ZTARG(5)
      DIMENSION CI(5),CJ(5)
      INTEGER ZIN,ZTARG,SYMB
      DIMENSION THICK(1)
C     THIS BLOCK OF WRITE STATEMENTS ARE USED ONLY IF THE CONCENTRATIONS
C     OF THE ELEMENTS ARE REQUIRED. CONCENTRATIONS ARE BEING CALCULATED
C     IN THE MAIN PROGRAM. SEE STATEMENT 600.
C     THIS ROUTINE CALCULATES THE CONSTANT  FOR EACH LAYER FOR EACH ELT
C     THE FORMULA ISCONSTANT = CONCEN * AVOGRADO NUMBER * THICKNESS
C     AVOGRADO NUMBER EQUAL 6.025*10**23.
      IF(ICON.EQ.0)GO TO 4005
      WRITE(6,1000)
1000  FORMAT(1H1)
      WRITE(6,4000)
4000  FORMAT(20X,100H**********************************************************
     **********************************************)
      WRITE(6,2000)
      WRITE(6,4001)
4001  FORMAT(60X,40HCONCENTRATION OF ELEMENTS(AT/CM2)/LAYER )
      WRITE(6,2000)
      WRITE(6,4000)
      WRITE(6,2000)
      WRITE(6,4002) (SYMB(ZTARG(K)),K=1,5)
4002  FORMAT(20H LAYER THICK(MG/CM2),7X,A2,22X,A2,21X,A2,21X,A2,24X,A2)
      WRITE(6,2000)
      WRITE(6,4003)
4003  FORMAT(20X,1X,5HCI(1),7X,5HCJ(1),7X,5HCI(2),7X,5HCJ(2),7X,5HCI(3),
     *7X,5HCJ(3),7X,5HCI(4),7X,5HCJ(4),7X,5HCI(5),7X,5HCJ(5))
      WRITE(6,2000)
2000  FORMAT(/)
      DO 1 I=1,5
      CI(I)=0.
1     CJ(I)=0.
      AVO=6.025 * (10.**23)
      DO 3 J=1,NLAYER
      DO 2 I=1,5
      CI(I)=CONCEN(I,J)*AVO*THICK(J)*.001
2     CJ(I)=CJ(I)+CI(I)
      WRITE(6,4) J,THICK(J),(CI(K),CJ(K),K=1,5)
4     FORMAT(1X,I4,3X,F4.2,4X,(5(2(1PE10.3,2X))))
3     CONTINUE
4005  CONTINUE
      RETURN
      END
```

## APPENDIX B - PROGRAM INPUTS

All inputs required to run PROFILE are listed in this appendix. Cards marked with * may require more than a single card.

| CARD | FIELD | DESCRIPTION |
|---|---|---|
| 1 | (20A4) | TITLE. A descriptive title for the calculation being done. |
| 2 | (10I1) | ISW(I),I=1,10. Sense Switches used to control calculations and outputs. 0 is off, 1 is on. See the listing of Subroutine Switch for description of each switch function. |
| 3 | (8F10.0) | CHAR, OMEGA. CHAR is the integrated beam change and OMEGA is the detector solid angle. These values are used if absolute fits are desired. |
| 4* | (8F10.0) | M1,M2,M3,M4,QREACT,EXCIT |
| 5 | (8510.0) | Blank.<br>This set of cards is used to define the reaction between the beam and target. There is a different 4 card for each target constituent, up to a maximum of five. A blank card ends the list of reaction cards. The reaction is defined as M2(M1,M3)M4 with QREACT being the reaction Q-value and EXCIT being the energy of excitation of a state in M4. |
| 6 | (8F10.0) | E,THETAT,THETAD,EMAX,EMIN,OTHET. This card defines the beam energy and target and detector geometries. E is the beam energy, EMAX and EMIN are the energy limits in MeV, over which the calculation is done, THETAD is the detector angle between target normal and beam and DTHET allows for a non-flat target surface where the beam hits it. |
| 7 | (8F10.0) | RS,DS,RT,RD and DD.<br>RS and DS define beam divergence, RD and DD define detector opening and RT is beam spot radius at the target. |

| CARD | FIELD | DESCRIPTION |
|---|---|---|
| 8 | (10I5) | NGS,NGT,NGD<br>Number of points used at the slit (NGS), target (NGT) and detector (NGD) to do the calculation. All are set to 1 unless large beam spots or detector apertures are used. |
| 9 | (8F10.0) | DETRES,ERES.<br>Resolution of the detector (DETRES) and beam energy (ERES) in keV. |
| 10 | (10I5) | NLAYER,NSLAB,NDIV.<br>NLAYER is the number of layers into which the target is divided, must be $\leq$ 100. NSLAB is the number of slabs into which the first layer is further subdivided. All layers are subdivided into the same thickness as the slabs of the first layer. NDIV is the number of points used to represent the outgoing particle Gaussian. |
| Inputs 11 through 13 are in Subroutine SETTAB. | | |
| 11 | (10I5) | ZIN(1), ZIN(2)<br>ZIN's are the atomic numbers of the incident (1) and outgoing (2) particles. |
| 12 | (10I5) | IZA, (ZTARG(I),I=1,5)<br>IZA is the number of target constituents<br>The ZTARG's are the atomic numbers of the constituents. |
| 13* | Unformatted | ATARG(I,K),K=1,NLAYER<br>ATARG(I,K) is the relative percentage of the element I in layer K. A new card must be used to begin the list for each element. I $\leq$ 5. |
| 14* | Unformatted | THICK (I), I=1, NLAYER<br>THICK's are the thickness (in $mg/cm^2$) of the layers. |
| Inputs 15 through 19 are in subroutine OUTPUT | | |
| 15 | (4F10.5) | XSC,YSFA<br>XSC is currently non-operative<br>YSFA is the Y-scale factor for printer plot, must be $\leq$ 120. |

| CARD | FIELD | DESCRIPTION |
|---|---|---|
| 16 | (4F10.5) | AY1,AY2<br>AY1 and AY2 are the lower and upper energy limits over which the least squares fitting is done. |
| 17 | (F8.0,1PER.5) | BIAS,CALX<br>Experimental energy spectrum parameters such that<br>E=*X-Bias)•CALX, where E is the energy and X is the experimental channel number. |
| 18 | (I5) | ICNT<br>ICNT gives the number of experimental data points to be input. ICNT ⩽ 400. |
| 19* | (10F8.0) | (X(I),Y(I),I=1,ICNT)<br>X and Y are the channel number and number of counts in that channel, respectively. |

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